PROCEEDINGS

10th EuChemS Chemistry Congress

12 - 16 July 2026 • Antwerp, Belgium

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Plenary Speakers

Spins in molecules: a versatile platform for quantum technologies

Roberta Sessoli
Department of Chemistry, University of Florence, Italy

A century after the birth of quantum mechanics, our understanding of matter has been profoundly transformed. The ability to harness fundamental quantum phenomena such as superposition and entanglement is now driving the so-called *second quantum revolution*. Alongside the impressive progress achieved with platforms such as superconducting circuits, cold atoms, Rydberg atoms, and photons, an important question emerges: Is there still room for alternative quantum platforms that could uniquely benefit from rational chemical design?

Spins—among the most elementary quantum systems—constitute the natural prototype of qubits, the building blocks of quantum computation. Their properties can be tuned through chemical design, making molecular spins particularly attractive platforms for quantum technologies. At the same time, spins also present challenges. Their weak coupling to the environment can lead to long coherence times, but it also makes single-spin manipulation and readout more demanding.

One promising route to overcome these limitations is the integration of spins with optical interfaces, as illustrated by the remarkable success of quantum technologies based on nitrogen-vacancy centers in diamond. Extending similar concepts to molecular systems requires new strategies that combine chemical design with advanced control schemes.

In this lecture, I will discuss our efforts to move in this direction by exploring a broader design space for molecular spin qubits, including photoactivated control mechanisms, spin–electric coupling, and the use of structural chirality for control and readout of molecular spins.

Masterpieces as chemical systems: unlocking the reactivity of art

Katrien Keune[1,2]
[1]Rijksmuseum, The Netherlands; [2]University of Amsterdam, The Netherlands

Paintings are dynamic chemical systems that, from the moment of their creation, undergo a wide range of chemical and physical changes that can ultimately alter their appearance and stability. Phenomena such as discolorations, the formation of disfiguring surface crusts, dramatically increased transparency, water sensitivity, paint embrittlement or the formation of protruding lead soaps aggregates are frequently encountered in historical oil paintings. Understanding the mechanisms and driving forces behind the ageing and degradation processes in oil paintings is highly challenging due to the complexity and heterogeneity of these systems.

To gain deeper insights, masterpieces undergo comprehensive chemical analyses spanning the macro- to nanoscale in one, two, and three dimensions. Techniques range from macro-X-ray fluorescence scanning (MA-XRF) and Reflectance Imaging Spectroscopy (RIS) to correlated X-ray fluorescence and ptychographic nano-tomography. Analyses begin with non-invasive methods and, where feasible, extend to invasive investigations. The results are interpreted in the context of the conservation history of the painting and historical documentation of painting materials.

Insights obtained from the examination of real paintings guide the design of chemically well-designed model systems, which are subsequently studied to target specific reactions or mechanisms. Understanding these processes is essential for predicting how aging and degradation phenomena may progress over time, as well as for assessing the impact of conservation treatments, display conditions, and storage environments. In addition, this research provides a more detailed understanding of the artists' creative processes. In this plenary lecture, examples will be presented from paintings by, among others, Rembrandt, Vermeer and Van Gogh.

Figure 1: 'The Night Watch' (1642) by Rembrandt van Rijn, Rijksmuseum, Amsterdam, The Netherlands. Daylight photo (leftside) and elemental map of lead (M-shell) taken with the MA-XRF. (credits image: Operation Night Watch team, Rijksmuseum, Amsterdam)

Soft Porous Crystals: Expanding the Paradigm of MOF Chemistry

Susumu Kitagawa
Kyoto University, Japan

For decades, functional materials have been designed under a central principle: rigidity defines performance. Dense and stable structures have been associated with key properties such as conductivity, magnetism, and mechanical strength, while structural flexibility has generally been regarded as a weakness. The emergence of metal–organic frameworks (MOFs) introduced the first paradigm shift by demonstrating that **precisely designed porous networks can be constructed at the molecular level**, establishing a platform for controlling space in crystalline materials. Building on this foundation, a second conceptual advance has emerged: **softness and structural dynamics can themselves generate function**. This lecture focuses on Soft Porous Crystals (SPCs),[1] which undergo reversible, stimulus-responsive structural transformations upon interaction with guest molecules. Unlike conventional porous materials with static architectures, SPCs exhibit dynamic behaviors, such as breathing and gate opening. In these systems, function is not solely defined by static structure, but arises from the interplay between flexibility and molecular recognition, enabling selective adsorption and responsive transport. These findings demonstrate that **crystalline order and structural softness can coexist**, challenging the traditional view of materials design. Recent advances further extend MOF chemistry toward hybrid systems,[2] where interface engineering enables the translation of dynamic molecular behavior into macroscopic functionality. This expanding paradigm—from designed frameworks to adaptive systems—opens new directions for addressing challenges in energy, environment, and beyond. It also suggests a broader shift in materials chemistry,[3] where **function emerges not only from structure, but from its ability to respond and adapt**.

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Remembering the lab in computational molecular material discovery

Kim Jelfs
Department of Chemistry, Imperial College London, London, United Kingdom

We have been developing computational software towards assisting in the discovery of molecular materials with targeted structures and properties. While initially we have focused upon porous molecular materials, we will also address the ways in which our approach is generalisable to other molecular materials and their applications, including as organic semiconductors or for photocatalysis. Our evolutionary algorithm automates the assembly of
hypothetical molecules from a library of precursors. Our approach has already suggested promising targets that have been synthetically realised. We have also examined the application of both supervised machine learning and explainable graph neural networks for the rapid prediction of porous molecules' properties. Finally, we have trained a model (the Materials Precursor Score, MPScore) to guide our predictions to select materials that have a high chance of being synthesisable in the laboratory. We will also discuss our experimental work to gather data for improved models. Our EPSRC AI hub for Chemistry's (AIchemy) goals and research will also be discussed.

Black Magic Chemistry: Functional Carbons replace noble metals, allow new reactions, and show enzyme-like properties

Markus Antonietti
Max Planck Institute of Colloids and Interfaces, Department of Colloid Chemistry, Research Campus Golm, Potsdam, Germany

In times of sustainability, Carbon materials with their high surface area and abundant functionality, best made from simple starting products, are a convincing choice. Here, the notation “carbon” is rather broad and includes a diversity of covalent organic compounds with different composition, architecture, textures and the related properties. A common denominator is however that all these systems are made by cross-linking processes to become insoluble, rather inert solids at elevated temperatures.
I will summarize in my talk some of our recent approaches to generate novel carbons, e.g. noble carbons, “oxocarbons” or P-carrying carbons, focusing on simplicity (the real sophistication)
I will show that many of the resulting 2d- and 3d structures are chemo-, photo- and electrocatalytically active, partly exceeding reference noble metal catalysts. Some special systems show even enzyme-like behavior for non-biological reactions, such as binding and conversion from nanomolar concentrations in complex media for environmental cleaning or polymer degradation of otherwise stable polymers.

Markus Antonietti is Director of the Max Planck Institute of Colloids and Interfaces and has contributed with about 1000 papers to the field of material/polymer chemistry in the last 35 years. His work was appreciated with a number of honours, and his current work is cited about 13000 times/year, with an H-index of 226. He is also active in fusion cuisine and is singer of a pub rock band.

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Award Speakers

Molecular mechanisms of water electrolysis: How to make green hydrogen

Marc Koper
Leiden Institute of Chemistry; Leiden University, Leiden, The Netherlands

The electrocatalytic hydrogen and oxygen evolution reactions are the cornerstone reactions of water electrolysis. I will discuss recent advances from my group in how electrode structure and the electrolyte composition determines the rate of these reactions. This complex interplay between electrode and electrolyte is currently still far from being completely understood. For the hydrogen evolution reaction (HER), cations play a key role in alkaline media in promoting or inhibiting the rate-determining step of HER. For the oxygen evolution reaction (OER) on NiFe-oxyhydroxide catalysts, cations have a strong effect on the non-kinetic contribution to the OER rate, suggesting that cations influence the accessibility of the active sites inside the layered oxyhydroxide. Finally, the electrolyte composition can have a major influence on bubble dynamics at high current densities, for both reactions.

Small molecule activation by electrocatalysis: Reduction of nitrogen to ammonia and valorization of carbon dioxide

Ronny Neumann
Dept. of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel

Introduction: Low temperature electrocatalytic reactions are an important toolbox for the development of sustainable transformations. Among these are the reduction of N_2 and CO_2 as important objectives toward the amelioration of global warming trends. In the realm of molecular electrocatalysis, the design of first row transition metal substituted polyoxometalates is a useful technique for small molecule activation.
Aim: The objective of this research was the activation of N_2 and CO_2 toward their selective cathodic reduction of N_2 and CO_2 to NH_3 and CO, respectively, through preparation of specifically designed polyoxometalates. The complementary anodic reaction is the oxidation of water as a source of protons and electrons, an important factor necessary for the achievement of sustainability.
Material and Methods: Polyoxometalates, notably $[SiFe_3(H_2O)_3W_9O_{37}]^{7-}$ $\{Fe_3W_9\}$ and $[SiCuFeGa(H_2O)_3W_9O_{37}]^{9-}$ $\{CuFeGaW_9\}$ were prepared and characterized. The activation of N_2 and CO_2 was studied by voltammetry coupled with IR, UV-Vis, Raman, and NMR techniques supported by calculations.
Results: (Figure) (1) N_2 to NH_3 reduction. N_2 activation was observed under cathodic bias by $\{Fe_3W_9\}$ in THF with Li^+ as promotor and in PEG with Na^+. Intermediates on the pathway from N_2 to NH_3 were observed by UV-vis and vibrational spectroscopies. Controlled potential spectroscopy showed formation of NH_3 using water as proton/electron donor in PEG/Na^+ reactions. (2) CO_2 to CO reduction. CO_2 activation and electrochemical reduction with $\{CuFeGaW_9\}$ was the best catalyst. Bimodal activity was observed with reaction optimal at -1.5 V and -2.5 V. Reaction intermediates were observed and DFT calculations were used to explain the divergent reaction pathways. Formation of CO was also coupled with anodic alkene epoxidation.
Conclusion: Activation of N_2 and CO_2 was shown by Cu and Fe based polyoxometalate catalysts as shown by voltametric measurements. Electrocatalysis was yielded the selective formation of NH_3 and CO. Valorization of CO_2 reduction was improved by alkene epoxidation.

Photocatalytic micromotors as programmable active materials

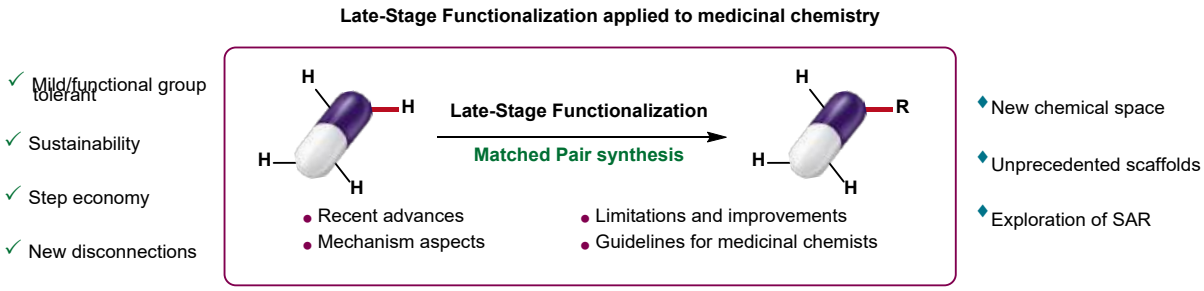
Katherina Villa Gómez
Institute of Chemical Research of Catalonia (ICIQ), Spain

The conversion of light into motion at microscopic scales is opening new opportunities for designing dynamic chemical systems that operate far from equilibrium. Photoactive micromotors represent a promising class of materials that harness photocatalytic reactions at semiconductor interfaces to generate self-propulsion and controllable interactions under light irradiation.
In this lecture, I will present our recent work on visible-light-driven micromotors based on inorganic semiconductors and metal–complex colloids. By designing particles with anisotropic morphologies and tailored surface chemistry, we develop systems with enhanced propulsion, selectivity and tunable optical responses.
Beyond propulsion, light can also be used to direct and organize these tiny motors. Using spatially patterned illumination, we can guide individual particles along predefined paths and control how they come together and assemble. This allows us to create dynamic structures that can be formed and reconfigured on demand.
Overall, these results demonstrate how photocatalytic processes at semiconductor interfaces can be exploited to control motion and collective behavior at the microscale, paving the way toward advanced strategies for micromanipulation, dynamic self-assembly, and light-driven catalytic systems.

HTE-enabled late-stage C–H functionalization - A toolbox for sustainable drug discovery chemistry

Magnus J. Johansson
AstraZeneca, Gothenburg, Sweden

Late-stage functionalization (LSF) is transforming pharmaceutical discovery by enabling direct, selective modification of complex drug-like molecules without rebuilding core scaffolds. This presentation will describe the work we have done at AstraZeneca over the last 10 years integrating high-throughput experimentation (HTE) with late-stage C–H functionalization to create a practical, sustainability-forward engine for analogue generation, accelerating SAR while reducing material use, solvent demand, and waste.
In drug discovery, LSF unlocks efficient diversification pathways for complex drug molecules through targeted activation of unfunctionalized C–H bonds in advanced intermediates. By avoiding lengthy *de novo* synthesis and eliminating the need for pre-installed reactive handles, this strategy enables precise molecular editing to enhance analogue potency, refine physicochemical/ADME properties, and expedite installation of chemical probes. From a green chemistry standpoint, LSF can reduce dramatically step count, including protecting-group manipulations, redox adjustments, and convergence detours that amplify material and energy demands. Fewer steps translate into lower process mass intensity (PMI) through reduced solvent volumes, excess reagent, byproduct formation, and purification burdens per kilogram of product. Collectively, this work establishes HTE-LSF as a paradigm where accelerated molecular innovation converges with environmental responsibility, proving that efficiency and sustainability are synergistic drivers in pharmaceutical research.



Teaching chemistry and conducting research in wartime Ukraine

Roman Gladyshevskii
Dept. of Inorganic Chemistry, Ivan Franko National University of Lviv, Ukraine

In February 2022, Russia launched a full-scale invasion of Ukraine. In spring 2026, the war goes on and universities, like the rest of society, have had to adapt. The presentation will focus on the Ivan Franko National University of Lviv (IFNUL), a classic university with 365 years of history, 19 faculties, and 25'000 students.

The war has strengthened the feeling of national unity and solidarity. Several volunteer centers operate at IFNUL and charity events are organized to collect funding for war victims.

Our aim is to propose high-quality education in a safe environment, so that our students and collaborators can stay in Ukraine and continue their activity under reasonable conditions. The working days are sometimes interrupted by air raid alarms, and the lectures are then continued in shelters. We observe that the level of knowledge of the students remains unchanged, but their motivation has increased.

Focus is on barrier-free education. The integration of the increasing number of war veterans and injured civilians will pose new challenges. To relieve the heavy psychological strains caused by the war, IFNUL has installed psychological services that offer individual consultations and various activities. The student associations play an important role.

The Russian missiles continuously attack the energy infrastructure and electricity has become a critical issue. IFNUL has installed conventional power supplies, solar hybrid stations, and batteries.

High priority is research on dual-use materials. Initiatives for collaboration have been launched in different countries, particularly in chemistry, physics, biology, IT-technology. One third of the research at IFNUL is financed by state funding, one third by international sources, and one third by industry and others. Technical and scientific equipment has been made available to researchers from across the country. The creation of startups is strongly encouraged, since the war will be followed by a period of intense reconstruction.

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Invited Speakers

APC - D1 - I01
Molecular structure identification in mass spectrometry by FEL-based Infrared ion spectroscopy

Debora Scuderi
Institut de Chimie Physique, UMR8000, CNRS-Université Paris Saclay, Orsay, France

Tandem mass spectrometry (MS/MS) is a key methodology to study biomolecules, with the electrospray ionisation (ESI) being one of the preferred ionization techniques [1]. It is well recognized as an efficient and highly versatile analytical tool [2], however its potential has long been limited by the structural information it can provide.
For this reason, the combination of tandem mass spectrometry with IR Multiple Photon Dissociation (IRMPD) spectroscopy has become a powerful tool for 3D structural characterisation of molecular ions in the gas phase [3].
Exploiting highly intense and widely tunable Free Electron Laser (FEL), IRMPD spectroscopy allows for the derivation of the vibrational fingerprint of molecular ions under tandem mass spectrometry (MS/MS) conditions [4]. Because resonant absorption of IR photons depends on molecular vibrations, the subsequent fragmentation event is highly structure specific, revealing characteristic functional groups of the molecule.
These kinds of experiments need to be performed with high power and widely tunable IR sources, i.e. free electrons lasers (FEL) at the FELIX (Free Electron Laser for Infrared eXperiment) facility in the Netherlands [5], and at the CLIO (Centre Laser Infrarouge d'Orsay) facility in France [6]. Their temporal structure and high brightness have been shown to be particularly suitable for inducing a rapid increase of the internal energy through an efficient resonant multiple photon absorption process [7]. Furthermore, they are easily tuneable in the mid-infrared region allowing for recording the IR spectra in the so-called IR fingerprint region.
Some applications of IRMPD spectroscopy are presented here to illustrate how it can be exploited to identify the oxidation site and the structures of model peptides containing methionine and DNA bases unravelling the relationship between the structure of the free radical formed during the first step of the oxidation process and the final compound [8].

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APC - D2 - I01
Advancing the chemical measurement science enterprise – A case for strengthening analytical chemistry education

Zoltan Mester
National Research Council, Canada

Analytical chemistry is the connective tissue on which the chemical sciences are built. Without reproducible, quantified observation of matter (analytical chemistry) modern chemistry would not exist as a coherent empirical science.
This presentation examines the chemical measurement science enterprise—from early assays to today's automated and AI-enabled laboratories—and shows why trustworthy measurements are essential for sound decisions in research, industry, and public policy.
Long before chemistry coalesced as a formal, conceptual science, societies interrogated material composition—effectively practicing what would later be called *analytical chemistry*. From touchstone methods and fire assays to high-resolution mass spectrometry, societal progress has relied on continual advances in chemical measurement science.
Physical measurements typically address a single, directly accessible quantity with a relatively simple traceability path. In contrast, chemical measurands are inherently contextual, requiring explicit definition of which species, in what form, in which matrix, and under what sampling and analytical conditions are being measured. The development, execution, and interpretation of such measurements demand highly trained chemical measurement scientists who can manage this complexity.
There is growing evidence that analytical chemistry is being eroded as a scientific discipline, shaped by faculty appointments, funding structures, and the perception of the field as merely a service function. At the same time, advances in instrumentation, software (including AI tools), and robotics have led some organizations to conclude, incorrectly, that the need for highly trained analytical specialists is diminishing. An emerging misalignment between university curricula and workplace needs contributes to longer onboarding and higher training costs, despite the fact that the most frequently used practical skills of chemistry graduates are in chemical analysis. This presentation will report on an IUPAC project [1] that documents the global status of analytical chemistry and current initiatives to address these challenges, culminating in a white paper to inform curriculum development, funding priorities, and hiring decisions.

APC - D3 - I01
Is chemometrics still needed in the age of artificial Intelligence?

Federico Marini
Dept. of Chemistry, Sapienza University of Rome, Italy

The rapid development of Artificial Intelligence (AI) and machine learning technologies is profoundly transforming analytical chemistry and data-driven science. Deep learning, foundation models, automated feature extraction, and increasingly sophisticated predictive algorithms are enabling the analysis of datasets of unprecedented size and complexity. As these approaches become more accessible and widely adopted, a fundamental question emerges: Is chemometrics still needed in the age of Artificial Intelligence?
This lecture will explore the evolving relationship between chemometrics and AI, examining both the opportunities and the challenges arising from the integration of modern machine learning approaches into analytical workflows. While AI methods have demonstrated remarkable predictive capabilities in applications ranging from spectroscopy and imaging to metabolomics, process monitoring, and digital twins, many of the fundamental challenges associated with analytical data remain unchanged. Issues such as experimental design, data quality, preprocessing, model validation, uncertainty estimation, interpretability, transferability, and robustness continue to play a critical role in determining whether a model can be trusted and successfully deployed in real-world applications.
The presentation will argue that chemometrics provides the methodological framework required to transform AI from a powerful computational tool into a reliable scientific instrument. Concepts that have long been central to chemometrics—including latent-variable modeling, multivariate experimental design, variable selection, model validation, and the distinction between correlation and causation—remain essential for ensuring that predictive models generate meaningful and reproducible knowledge rather than merely accurate predictions.
Through examples drawn from analytical chemistry, spectroscopy, hyperspectral imaging, food authentication, forensic science, and multi-omics studies, the lecture will discuss how chemometric thinking can complement modern AI approaches and help address current concerns related to explainability, trustworthiness, and regulatory acceptance. Particular emphasis will be placed on the role of chemometrics in developing interpretable and scientifically grounded AI systems capable of supporting decision-making in complex analytical scenarios.
Rather than viewing chemometrics and AI as competing paradigms, the lecture will propose a vision in which they represent complementary components of a unified data-science framework. In this perspective, AI provides unprecedented modeling flexibility and computational power, while chemometrics contributes the scientific rigor necessary to ensure that analytical models remain robust, interpretable, and fit for purpose. The central question, therefore, may not be whether chemometrics is still needed, but whether Artificial Intelligence can fully realize its potential in analytical chemistry without it

APC - D4 - I01
Using novel adsorption phenomena for the characterization of nanoporous materials

Martin Oschatz
Institute for Technical Chemistry and Environmental Chemistry, Friedrich-Schiller-University Jena, Jena, Germany; Center for Energy and Environmental Chemistry Jena (CEEC Jena), Jena, Germany; Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Jena, Germany

Nanoporous carbon materials play an ever-increasing role in various fields like gas purification, energy storage, and catalysis.[1] In all of them, adsorption phenomena on the carbon surface are crucial steps. It is well known that the adsorption properties of such materials are a function of their pore architecture.[2] Pore size, pore geometry, pore connectivity, and pore hierarchy determine important factors like mass transport and the strength of interaction with different guest species.
Another (and possibly even more powerful) “regulation screw” to control the adsorption properties of nanoporous carbon materials is their atomic construction.[3] The controlled integration of heteroatoms (most often nonmetallic group III or group V and VI elements with nitrogen being the most widely studied heteroatom) into porous sp^2-based carbon networks can significantly change their physicochemical properties.
This contribution will focus on nitrogen-rich porous carbon materials with zeolite-like adsorption properties.[2,4,5] On the one side, gas physisorption and spectroscopic methods for their structural characterization beyond nitrogen and argon sorption will be discussed. Special focus will be on the water vapor sorption properties of such highly hydrophilic carbon-based materials. The method of thermal response measurements will also be presented and discussed. In addition to these fundamental characterization tools, the application of these porous nitrogen-rich carbon materials in CO_2 capture and hydrogen storage will be presented from a physicochemical perspective.

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CAI - D2 - I01
Accelerating chemical science in the era of LLMs

Phillipe Schwaller
Laboratory of Artificial Chemical Intelligence (LIAC), Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland; National Centre of Competence in Research (NCCR) Catalysis, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Introduction: Chemistry faces a fundamental challenge: the space of possible molecules and materials is nearly infinite, yet discovering useful new ones requires navigating costly cycles of design, synthesis, and testing. Large language models (LLMs), the same technology behind modern AI assistants, can be adapted to "speak" the language of chemistry and accelerate this discovery process.
Aim: We show how language models — from small, specialized molecular generators to general-purpose LLMs — can be adapted to propose synthesizable molecules, reason about synthetic routes, and guide experimental optimization across diverse scientific domains with minimal data.
Material and Methods: We present three complementary approaches: (i) reinforcement learning on a pre-trained generalist molecular generative model to propose novel molecules atom by atom while respecting reaction-based synthesizability constraints[1]; (ii) LLM-guided search frameworks (Synthegy) that integrate chemical reasoning with traditional retrosynthesis and mechanism elucidation tools[2]; and (iii) uncertainty-aware fine-tuning of LLMs to act as calibrated optimizers steered by natural-language descriptions of experimental conditions[3].
Results: Our generative framework loosely mimics virtual screening of ultra-large make-on-demand libraries: using only a single GPU, we generate and dock 15k molecules against Freedom 4.0 (142B make-on-demand molecules), with >90% exact match to imposed reaction constraints[1]. Synthegy achieves 71% alignment with 36 expert chemists on strategy-aware retrosynthesis and recovers plausible reaction mechanisms from elementary electron-pushing steps[2]. Across 19 optimization problems spanning organic synthesis, materials science, catalysis, process chemistry, and molecular design, our LLM-based optimizer ranks first on average, nearly doubling the discovery rate of high-yielding Buchwald–Hartwig conditions from 24% to 43% within 50 iterations[3].
Conclusion: Together, these advances illustrate how language models, when adapted and integrated with traditional chemical tools, can help scientists explore chemical space faster and more creatively, accelerating discovery from drug design to materials science.

Acknowledgements: This work was supported by the NCCR Catalysis (grant number 180544), a National Centre of Competence in Research funded by the Swiss National Science Foundation. We thank the members of the LIAC and our collaborators for their contributions.

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CAI - D3 - I01
Hierarchical integration of data science in materials research

Rigoberto Hernandez
Johns Hopkins University, USA

Chemistry and materials research increasingly blends scientific insight with data-driven methods. The hierarchy of integration between them provides a framework for the use of data science. At level one, machine learning can be used to replace computationally expensive calculations within the overall workflow. Examples included the determination of molecular forces needed to integrate molecular dynamics, and the determination of multidimensional non-recrossing dividing surfaces to calculate transition state theory rates.[1] At level two, data science can be used to predict overall properties without reference to any intermediate quantities. Examples include our recent determination of nanoparticle features to their effects on organismal viability through the use of ensemble methods suited to small datasets.[2,3] At level three, the learning model is engineered to reflect the system itself. For example, we can predict electronic band gaps using nested autoencoders that capture features and labels across multiple length scales at once.[4] At level four, physics-based theory and simulation are coupled seamlessly with data-science workflows in closed loops. While deeper integration feels natural to chemists, it can seem at odds with data-science practices that ``let the data speak'' without prior assumptions. Through the integration hierarchy, we show how to best reconcile domain science within data science approaches to accelerate reliable molecular and materials discovery.

We acknowledge support from the US National Science Foundation through Grant Nos. CHE-2001611 and CHE-210455.

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CBF - D1 - I01
Food fraud and countermeasures

Markes Fischer
Hamburg School of Food Science, Institute of Food Chemistry, University of Hamburg, Germany

Globally, food fraud most commonly affects products such as olive oil, fish, and organic foods, as well as raw materials like spices, tea, cocoa, coffee, and nuts. The global turnover from counterfeit or adulterated raw materials and foods amounts to several billion euros per year. This figure makes it clear that the quality control strategies employed to date are not up to the task. Compared to past centuries, today's challenges are far more complex and, due to global material cycles, involve determining the type of raw material (e.g., variety), identifying the exact geographical origin (e.g., to verify a product as a regionally protected food), and distinguishing between specific production methods (organic and sustainable vs. conventional agriculture). The presentation will provide insights into the latest approaches for experimentally verifying the authenticity of food ingredients.

Projects in the field of "food authentication" were funded by the Federal Ministry of Food and Agriculture (BMEL) through the Federal Office for Agriculture and Food (BLE), as well as under the "Industrial Collaborative Research" (IGF) program of the Federal Ministry for Economic Affairs and Climate Action (BMWK).

CBF - D2 - I01
Ligand-directed chemistry profiling of carbohydrate processing enzymes

Tanja Wrodnigg
Graz University of Technology, Institute of Chemistry and Technology of Biobased Systems, Austria

Activity-based protein profiling (ABPP) is a versatile tool for evaluating the activity of enzymes in living systems and complex environments rather than their abundance [1]. Several versatile and efficient ABPP strategies have been introduced with respect to carbohydrate processing enzymes (CPEs) [2]. A key feature of most of these strategies is that the enzyme is labelled by the covalent binding of the probe to the active site. We are interested in employing ligand-directed chemistry (LDC), introduced by Hamachi et al. [3], as a complementary method to label CPEs. This strategy enables labelling of the enzyme in close proximity to the active site, thereby allowing its intrinsic activity to be restored to a certain extent.
We have designed and synthesised glycomimetic-based probes that feature the components necessary for LDC labelling [4]. The biological activity of these probes has been evaluated using a selected panel of glycoside hydrolases.
Details on the synthetic approach for glycomimetic-based probes as well as results from their biological evaluation for LCD labelling of CPEs will be presented.

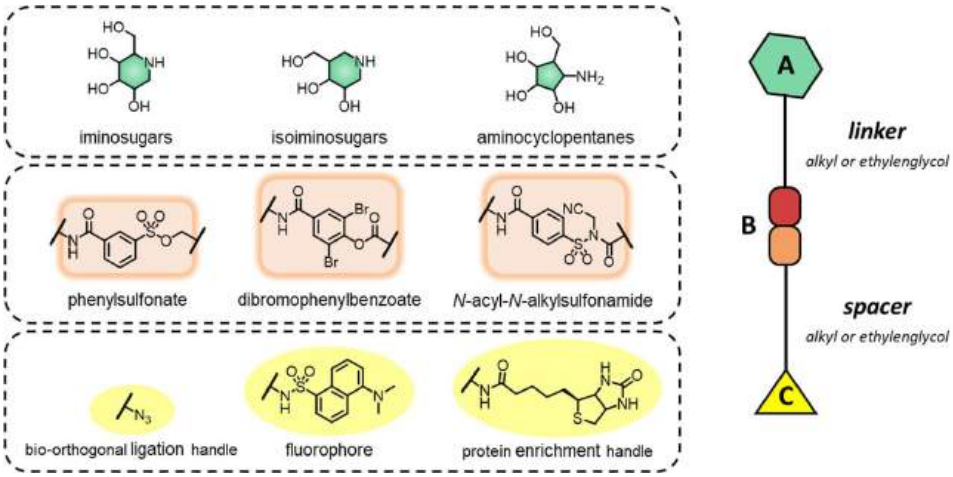

Fig. 1: Building block concept for ligand directed chemistry (LDC) probes targeting glycoside hydrolases. (A) reversible inhibitor as ligand; (B) linker with electrophilic reactive group; (C) reporter tag.

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CBF - D4 - I01
Carbohydrates as building blocks of structure in plant foods

Laura Roman Rivas
InnograinLab, Food Technology Division, Dept. of Agricultural Engineering, University of Valladolid, Spain; Institute of Sustainable Processes, University of Valladolid, Spain

Plant-derived carbohydrates, particularly starch polysaccharides, are major contributors to the human diet, playing a central role in the structure formation and nutritional implications of many plant-based foods. Meeting current nutritional and sustainability challenges requires a deeper understanding of how these dietary carbohydrates are structured and how their molecular and supramolecular motifs govern technological performance in food systems and in biological contexts, fostering high-quality and more nutritious diets. The inherent molecular and hierarchical complexity of these plant polysaccharides drives their functionality, while also posing significant analytical and processing challenges, especially when new plant sources and more sustainable processing technologies are involved. Carbohydrates are essential building blocks for creating the aerated and gelled structures typical of many extruded and baked cereal-based foods, while their nutritional relevance continues to raise questions about carbohydrate quality and health. In this presentation, particular attention is given to deciphering the hierarchical structure of energy-storage carbohydrates, their colloidal state and interactions with other plant components, and their functionalization through oriented processing into biomaterials for food and other applications involving the human body. I will emphasize the much-needed multidisciplinary analytical techniques for their study, including advanced chromatographic (coupled to enzymatic fingerprinting), microscopic, thermo-rheological, calorimetric and spectroscopic tools. Using a multidisciplinary analytical approach, this presentation aims to clarify how polysaccharides' hierarchical structure (from unit and internal chain length distribution) and processing conditions impact food material properties and aging, and links to digestion outcomes, providing mechanistic understanding of structure-function-digestion relationships.

Laura Roman would like to acknowledge financial support from the Ramón y Cajal program (RYC2021-032926-I), funded by MICIU/AEI/10.13039/501100011033 and the European Union "NextGenerationEU/PRTR", the Knowledge Generation Project (PID2022-139425OA-I00), funded by MICIU/AEI/10.13039/501100011033 and FEDER, EU and the Applied Research Project (VA157P24), co-funded by Junta de Castilla y León and FEDER, EU. L.R. also acknowledges the travel scholarship from Banco Santander Open Academy.

CCS - D1 - I01
Operando spectroscopy of heterogeneous catalysts to make fuels and chemicals from renewable resources

Bert Weckhuysen
Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry, Dept. of Chemistry, Faculty of Science, Utrecht University, Utrecht, The Netherlands

As we enter the era of catalytic activation of small molecules, such as CO_2, to realize the refinery of the future one of the main questions to answer for scientists involve the coupling of carbon fragments, originating from CO_2, either produced at point sources, or harvested from direct air capture units. The goal is to manufacture increasingly complex carbon-containing molecules from CO_2 – or the related molecule CO - instead of making them from crude oil fractions. This requires a profound knowledge of the chemical processes taking place at the catalytic surface of both thermo- and electrocatalytic activation processes of CO_2, was well as of the subsequent chemical conversion processes in which carbon monoxide (Fischer-Tropsch synthesis), methane (via C-H activation to make e.g. olefins and aromatics) and methanol (methanol-to-hydrocarbons process) are used. This is the topic of this lecture, in which the latest progress made in our research group will be discussed in understanding CO_2 activation over nickel (thermocatalytic conversion) as well as copper (electrocatalytic conversion), and the subsequent conversion processes of the reaction products to make fuels and chemicals, including long-chain hydrocarbons, methanol and aromatics, thereby making use of combination catalysts as well as processes. Special emphasis is on the use of operando spectroscopy methods to elucidate reaction and deactivation mechanisms. The last part of the talk will be focused on alternative resources, namely plastic waste, thereby illustrating the issue of mass transfer processes, as well as the role of active sites embedded at the outer surface of solid catalysts, to ensure for example pre-cracking of the large hydrocarbon molecules. The focus here will be on the use of fluid catalytic cracking (FCC) technology to convert plastic waste into base chemicals, as well as on the characterization of surface acid sites at the outer surface, and their role in the cracking of long-chain hydrocarbons, and other parameters to describe the behavior of FCC technology to convert plastic waste into fuels and chemicals.

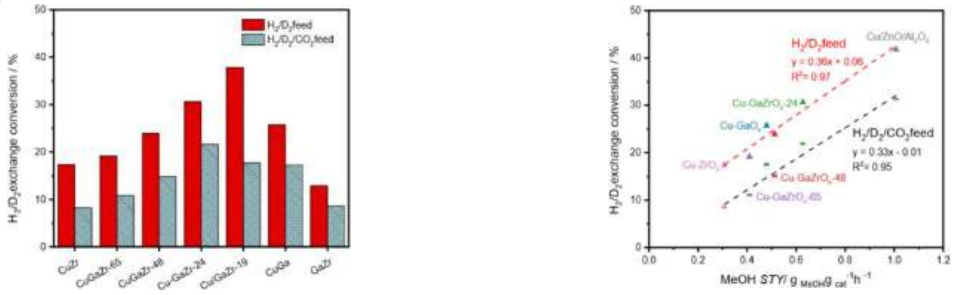
CCS - D2 - I01
Detangling complex catalytic systems for sustainable transformation

Ive Hermans
The Johns Hopkins University, Baltimore, MD, USA

Introduction: Developing sustainable catalytic processes requires a deep understanding of heterogeneous systems that often combine multiple active components and dynamically evolving surface chemistry. In such systems, reaction intermediates may coexist with spectator species, and rate-determining steps can change with operating conditions. As a result, extracting mechanistic insight from complex catalytic networks remains a major challenge. Although steady-state characterization and kinetic measurements provide valuable foundational knowledge, they frequently lack the temporal resolution necessary to disentangle intertwined reaction pathways under realistic conditions.
In this work, CO2 hydrogenation to methanol is employed as a representative reaction to demonstrate a structured methodology for interrogating complex catalytic systems. Initial insight is obtained through conventional catalyst synthesis, reactor evaluation, and probe reactions, which establish macroscopic structure–performance relationships. Nevertheless, despite decades of study on Cu-based methanol synthesis catalysts, fundamental questions persist concerning the nature of reactive intermediates, the function of promoters, and the origins of pressure-dependent kinetic behavior [2,3].
To overcome these limitations, we show that in-situ Modulation Excitation Spectroscopy (MES) provides a decisive layer of mechanistic resolution. By periodically perturbing the reactant feed and analyzing the system response via phase-sensitive detection, MES isolates signals arising exclusively from actively participating surface species and exposes changes in the catalytic sequence as a function of pressure. Using ternary $CuGaZrO_x$ catalysts as a model system, this study illustrates how dynamic operando spectroscopy augments traditional approaches to systematically resolve complex catalytic mechanisms [1].
Materials and Methods: Ternary $CuGaZrO_x$ catalysts were prepared by coprecipitation while maintaining a constant Cu loading (~20 wt%) and systematically varying the Ga/Zr ratio, resulting in amorphous materials with intimate metal–oxide mixing previously shown to favor methanol formation [1]. Catalytic performance was assessed in a fixed-bed flow reactor operated at 35–50 bar and temperatures between 220 and 280 °C, with product streams analyzed by online gas chromatography.
Operando modulation excitation DRIFTS measurements were carried out under reaction conditions by periodically modulating the CO2 feed while keeping total flow and pressure constant. Phase-sensitive analysis of the infrared response enabled extraction of amplitudes, harmonics, and phase delays associated with dynamically responsive surface species. These spectroscopic experiments were complemented by reaction order measurements and H2/D2 isotopic exchange studies to evaluate hydrogen activation and availability [1]. All abbreviations are defined at first mention.
Results and Discussion: Operando MES measurements reveal that CO2 hydrogenation over $CuGaZrO_x$ catalysts primarily follows a formate-based reaction pathway, with surface methoxy species emerging as immediate precursors to methanol formation. Phase-resolved ME-DRIFTS spectra shows that both formate and methoxy signals respond synchronously to periodic feed modulation, providing direct evidence that these species participate actively in the catalytic cycle rather than acting as spectators. While consistent with prior mechanistic hypotheses for Cu-based catalysts, these results offer direct validation under industrially relevant pressures [2,3].
Analysis of phase delays demonstrates that the temporal relationship between formate and methoxy intermediates evolves with pressure and temperature, indicating a shift in the kinetically controlling step along the hydrogenation sequence. Independent kinetic measurements show that methanol formation is first order in H_2 and exhibits a negative dependence on CO2 partial pressure, pointing to a hydrogen-limited regime [1].
This conclusion is reinforced by H2/D2 exchange experiments, which reveal a linear correlation between methanol space-time yield and hydrogen scrambling rates, identifying hydrogen activation as a key kinetic descriptor [1]. MES further confirms that the transformation of formate-derived intermediates is strongly coupled with hydrogen availability.

At higher pressures, the conversion of methoxy species to methanol proceeds through a water-assisted step, as evidenced by correlated dynamic responses of surface methoxy species, gas-phase methanol, and water. Incorporation of Ga selectively stabilizes hydrogen-rich surface intermediates and suppresses kinetically favorable pathways to CO by increasing the apparent barrier for the reverse water–gas shift reaction [1]. Together, these observations bridge reactor-scale kinetics with molecular-level dynamics and underscore the necessity of time-resolved operando techniques for capturing the true catalytic mechanism.

Fig. 1: The left panel shows the H2/D2 exchange conversion on CuGaZrOx samples at 140 oC and 6 bar using inlet composition of (20% H2/ 20% D2/ Ar) and (20% H2/ 20% D2/ 10% CO2/ Ar). The right panel shows H2/D2 exchange conversion as a function of the methanol STY on the coprecipitated CuGaZrOx samples as well as the industrial Cu/ZnO/Al2O3



Significance: This study highlights how dynamic operando spectroscopy at industrially relevant pressures enables mechanistic insight that cannot be obtained from steady-state measurements alone. By explicitly linking hydrogen activation, surface intermediate dynamics, and product formation, the approach presented here provides generalizable design principles for methanol synthesis catalysts and demonstrates the broader utility of MES for unraveling complex heterogeneous catalytic systems.

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EES - D1 - I01

In situ reaction monitoring, molecular dynamics simulations and machine-learning-augmented data analysis in deciphering mechanochemical transformations

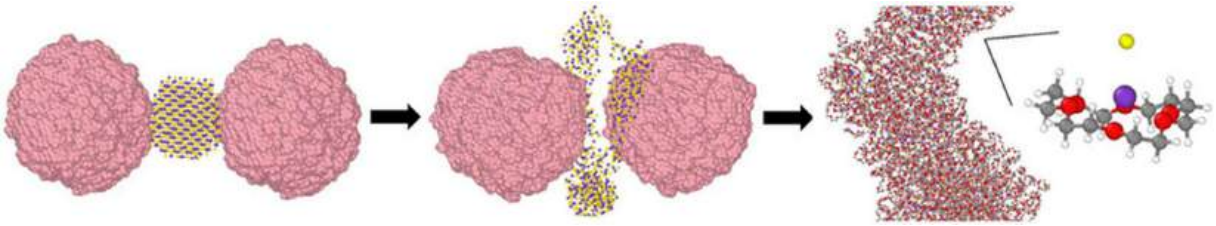
Ivan Halasz
Ruđer Bošković Institute, Zagreb, Croatia

Abstract

Mechanochemistry has emerged as a powerful approach to sustainable chemical synthesis, yet the molecular-level mechanisms by which mechanical impacts drive chemical transformations remain incompletely understood.[1] Over the past decade, in situ powder X-ray diffraction (PXRD) and Raman spectroscopy have transformed mechanochemical studies from largely qualitative observations into time-resolved analyses of bulk structural and molecular change. These methods have revealed highly dynamic reaction environments in which transformations can occur within minutes, transient intermediates are frequently observed, and reaction pathways can be controlled through liquid additives, catalysis, or the solid forms of starting materials.[2] However, limitations in time resolution, sample averaging, and data quality still constrain mechanistic interpretation, particularly under realistic milling conditions.

This contribution discusses how mechanochemical transformations can be deciphered through the integration of in situ reaction monitoring, molecular dynamics simulations, and machine-learning-augmented data analysis. Using the model reaction between potassium chloride and 18-crown-6 ether, molecular dynamics simulations provide a collision-level description of reactivity, showing that product formation is initiated by collision-induced fragmentation of the KCl crystal when the absorbed energy per ion pair exceeds the crystal cohesion energy.[3] Complex formation follows this fragmentation step, while water acts as a liquid additive with a non-linear effect: small amounts promote complex formation, whereas excess water stabilizes the reactants and suppresses reactivity.

Together, these findings connect macroscopic time-resolved experimental observations with molecular-scale descriptions of individual milling events. Looking forward, machine-learning methods offer a route to improve the analysis of time-resolved PXRD data, especially where experimental conditions prioritize temporal resolution over spectral or diffraction quality.[4] By combining in situ monitoring, simulation, and advanced data analysis, mechanochemistry can move toward a more predictive framework for understanding reaction mechanisms and rationally optimizing milling conditions, including the selection and dosing of liquid additives.



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IM - D1 - I01
Porous materials for biohybrid systems: metal-azolate framework biocomposites.

Paolo Falcaro[1]
[1]*Graz University of Technology, Graz, Austria.*

Metal-Azolate Frameworks (MAFs) can be combined with biomimetic mineralization strategies, thereby demonstrating the capacity to spontaneously form a protective coating around sensitive biomacromolecules and their assemblies. Different reports show that distinct crystalline phases can be prepared under varying synthetic conditions, and each phase exhibits distinct functional properties. Motivated by these observations, we systematically explored a substantial portion of the viable reaction space to establish an extended map of the domains of the most prominent Zeolitic Imidazolate Framework, ZIF-8. By varying precursor ratios, overall concentrations, and post-synthetic treatments, we constructed ternary phase diagrams that reveal how crystallinity, porosity, encapsulation efficiency, and loading capacity depend on the resulting phase. Then we examine the influence of a mixed-ligand approach on the preparation of enzyme@MAF systems. Overall, this progress establishes a foundation for the informed design of MAF biocomposites with tunable structure and properties for drug delivery and biocatalysis.

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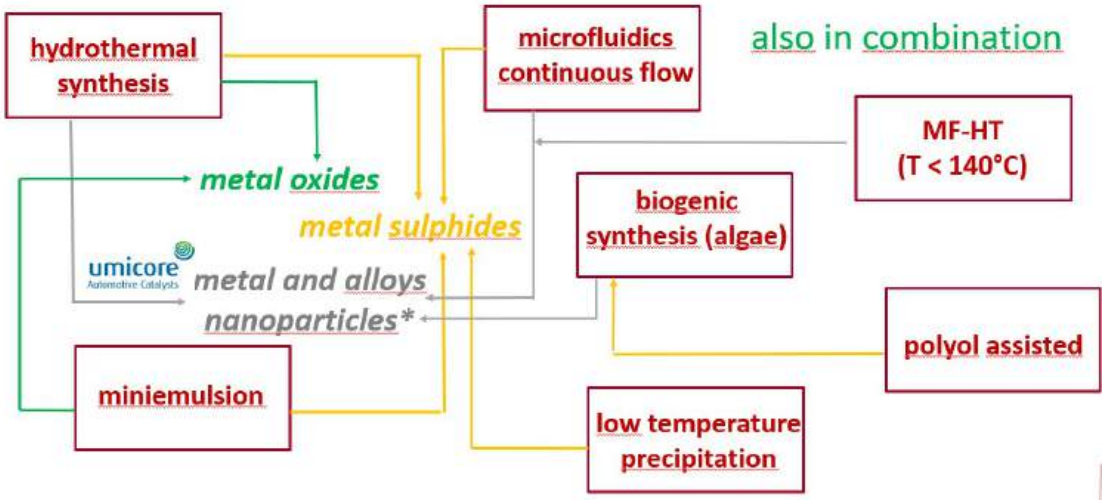
IM - D2 - I01

Sustainable inorganic materials chemistry: Tools and boundaries to rationally navigate the experimental parameters space

Silvia Gross
Dept. of Chemical Sciences, University of Padova, Italy and Institute for Chemical Technology and Polymer Chemistry (ITCP) – Karlsruhe Institute of Technology (KIT), Germany

Introduction: A careful materials selection and the optimisation of efficient, low-cost and environmentally friendly advanced inorganic materials for functional applications such as environmental protection, energy conversion and storage and catalysis are paramount to target sustainable synthesis in a zero-emission and in a critical raw materials perspective.
Aim: Inorganic materials synthesis should however comply not only with the paradigms of *green chemistry*, as well as with these of its more recent implementation, *circular chemistry*, but also with further synthetic requirements. Low temperature of processing, use of benign and not hazardous and earth abundant precursors, use of water or not toxic/not flammable solvents, high yields, low energy and materials consumption, easy implementation at industrial scale, reproducibility are only some of the basic requirements to be met. In this context inorganic materials chemistry represents an exciting playground for the design and optimisation of sustainable routes, and the resort to unconventional synthesis conditions discloses exciting perspectives in orienting, inter alia, the size, the morphology and the final structure of the crystalline materials. A valuable support can derive from the application of statistical or theoretical tools, enabling to rationalise the synthetic path and to minimise the experimental effort and the related energy and materials consumption.
Material and Methods: In this framework, in our group at University of Padua we have explored different low (T< 150°C) temperature and sustainable wet chemistry and colloidal routes to produce size- and shape-controlled inorganic nanomaterials for heterogeneous catalysis, gas exhaust abatement, energy storage. (Fig.1). For most of them, an extensive exploration of the experimental parameters space was accomplished by a systematic and controlled variation of the different involved variables, also supported by Design of Experiments.



Results: By exploiting unconventional experimental conditions disclosed by the different methods, i.e. not standard temperature and pressure or the confined space inside the miniemulsion-generated droplets, we prepared ferrites, manganites, pure and doped metal oxides, sulphides, halogenides, metal/metal oxide nanocomposites, supported metal nanoparticles and, recently, high entropy spinel oxides, with up to 7 cations. These latter systems have been shown to have interesting catalytic properties in OER.
Conclusions: Exciting results could be achieved by the combination of the above-mentioned routes and by a systematic exploration of the broad parameters landscape.

Acknowledgements: Silvia Gross gratefully thanks the University of Padova, DFG for a Mercator Fellowship within the SFB Project TrackAct (2024-2028) and the Justus Liebig University of Giessen for an honorary Liebig-Professorship.

IM - D3 - I01
Engineering local chemical environments for efficient aqueous batteries

Maria Lukatskaya
Dept. of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

Electrolyte structure dictates interfacial speciation, transport, and reaction kinetics in electrochemical energy storage systems. In aqueous batteries, these relationships define the electrochemical stability window, interfacial reactivity, and metal deposition behavior. This work examines how local chemical environments, set by ion coordination, solvation structure, intermolecular interactions, and the resulting interfacial speciation, govern these processes and can be engineered to improve performance.
Water-in-salt (WIS) electrolytes have enabled aqueous batteries with expanded stability windows and compatibility with high-voltage electrode materials. Beyond highly concentrated systems, similar behavior can be achieved using mixed-cation and coordinating-anion chemistries, providing access to WIS-like environments with improved cost and sustainability. These systems highlight the role of ion coordination and solvation structure in defining electrolyte properties and interfacial behavior.
The mechanistic origin of the expanded stability window is examined through hydrogen evolution reaction (HER) kinetics. Suppression of HER in WIS systems does not arise primarily from reduced bulk water activity. Instead, disruption of the hydrogen-bonding network decreases interfacial water availability, while slow water transport within the electrical double layer limits reactant replenishment. A direct correlation between interfacial water coverage and HER exchange current density identifies interfacial water structure and transport as rate-limiting factors.
These insights are extended to aqueous Zn metal batteries, where electrolyte structure governs ion transport, interfacial speciation, and deposition behavior. WIS-like Zn^{2+} coordination environments can be achieved in relatively dilute electrolytes through the use of coordinating anions, shifting solvation from water-dominated to anion-rich environments without the transport limitations of highly concentrated systems. This enables improved conductivity, reduced overpotentials, and more stable Zn deposition. Anion–cation interaction strength emerges as a key parameter controlling deposition kinetics and morphology.

IM - D4 - I01

When CO_2 replaces isocyanates in polyurethane foams: From rapid room-temperature self-blowing processing to end-of-life solutions

Bruno Grignard[1,2], Christophe Detrembleur[1,3], Maxime Bourguignon[1], Victor Lechuga-Islas[1], Emmeline Gillissen

[1]CO_2 technology Platform, FRITCO$_2$T, University of Liege, Liege, Belgium; [2]Center for Education and Research on Macromolecules (CERM), CESAM Research Unit, University of Liege, Liege, Belgium; [3]WEL Research Institute, Wavre, Belgium

Over the past 80 years, polyurethane (PU) foams have profoundly transformed our modern life, finding applications in insulation, comfort materials (e.g., footwear, mattresses, impact protection), biomedical devices… In conventional PU systems, foaming arises from the in situ generation of CO_2 through isocyanate hydrolysis during reactions with polyols, leading to lightweight porous structures. However, the vast majority of commercially available PU foams still rely on fossil-based polyols and toxic isocyanates. In response to increasing demands for circularity and resource efficiency, industrial efforts—such as those by Covestro—have enabled the incorporation of captured CO_2 into polyols, reducing the carbon footprint of flexible PU foams. Despite this progress, these materials still depend on hazardous polyisocyanates, some of them being subjected to regulatory restrictions under REACH. Consequently, there is a strong impetus to develop safer, isocyanate-free alternatives while also addressing end-of-life considerations.

In this contribution, we present a straightforward and cost-effective strategy to produce CO_2 self-blowing non-isocyanate polyurethane (NIPU) foams that replicate conventional foaming mechanisms by using water as a chemical blowing agent. The NIPU matrix is synthesized via the copolymerization of polyamines with polycyclic carbonates, the latter being readily accessible at multi-kilogram scale through the coupling of CO_2 with epoxides. We demonstrate that this self-foaming process can be tuned to meet industrial requirements, enabling rapid foam formation (3–10 minutes) from solvent-free formulations at ambient temperature.[1] This approach offers strong potential for retrofitting existing industrial infrastructures. Furthermore, end-of-life strategies for NIPU foams are explored through chemical recycling, yielding products suitable for the production of second-generation foams. In parallel, the covalent adaptable network (CAN) nature of NIPUs is leveraged to upcycle these thermoset materials into reprocessable, second-life adhesives exhibiting performances comparable to commercial counterparts.[2]

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MDR - D1 - I01
Chiral metallacrown complexes

Alexander Hagenow[1], David Anthofer[2], A. Wittmann[2], H.-J. Elmers[2], E. Rentschler[1]
[1]Dept. Chemie, Johannes Gutenberg-Universität, Mainz, Germany; [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

The discovery that structural chirality can induce strong spin polarization challenges the conventional assumption of how spin filtering arises. This discovery has significant implications for chemistry and biology, as it could affect reaction rates and biological function.
We have designed molecules with different geometries to introduce chirality into molecular magnetic materials. In particular, we focus on the unique chemical and structural features of molecules in the metallacrown family. Metallacrown complexes (MCs), which consist of metal ions and bridging ligands that self-assemble into cyclic ring structures, offer a particularly promising approach. Their atomic configurations enable tunable magnetic exchange between metal ions within the ring, providing a basis for improving SMM properties by incorporating ions with pronounced magnetic anisotropy. In an innovative approach, we combine the synthesis of magnetically interesting metallacrowns with advanced methods to study the molecular systems on the surface.[1-3]

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MDR - D3 - I01
Chirality related properties in molecular materials

Narcis Avarvari
University of Angers, CNRS, MOLTECH-Anjou Laboratory, Angers, France

Chirality manifests itself in many areas of physics, chemistry and biology, where objects or materials can exist in two non super-imposable forms, one being the mirror image of the other. In this respect, chiral materials[1] are gaining continuous interest in the frame of chirality related physical phenomena such as the circularly polarized luminescence (CPL), electrical magnetochiral anisotropy (eMChA) effect or the chirality induced spin selectivity (CISS) effect. The eMChA effect expresses the dependence of the resistance of a chiral conductor on its handedness and on both the relative orientation of the electrical current and the applied magnetic field,[2] whereas the CISS effect refers to the selective transmission of a preferential electron spin orientation through a chiral material.[3] In this contribution we will discuss the occurrence of these phenomena in chiral tetrathiafulvalenes (TTF)[4,5] and helicenes.[6,7]

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High-Throughput Experimentation at Johnson & Johnson Process & Development: From Robotic Integration to Rapid Optimization

Florian Medina[1]

[1] Janssen Research and Development, A Division of Janssen Pharmaceutica NV, (A Johnson and Johnson Company), Turnhoutseweg 30, 2340 Beerse, Belgium

This presentation provides a glimpse into the Johnson & Johnson Chemical Process Research & Development High-Throughput Experimentation (CPRD-HTE) team and its integrated automation platform, highlighting how advanced hardware, data workflows, and modeling accelerate process development.

The first section will describe a part of the laboratory layout and some core capabilities. Key features include: (1) custom hydrogenation equipment combined with an end-to-end workflow for generating high-quality datasets to train machine-learning models that predict enantioselective catalytic outcomes;[1] and (2) in-house prototyping and integration of novel hardware solutions, such as near-infrared (NIR) sensors for real-time reaction profiling and a new solid-dosing platform that leverages a substantially larger chemical library to increase experimental throughput.

The second section presents a detailed case study demonstrating how HTE workflows are applied across a spectrum of projects — from routine transformations to complex palladium-catalyzed cross-coupling sequences — to shorten development timelines and improve decision quality. Examples will illustrate how miniaturization, parallelization, and rapid data analysis enable efficient condition screening, reaction understanding, and translational scale-up planning for active pharmaceutical ingredient (API) synthesis.[2]

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RC - D1 - I01
Responsible chemistry for society: From what chemistry can do, to what chemists should do

Peter G. Mahaffy
The King's University and King's Centre for Visualization in Science, Edmonton, Canada

As the profession focused on the transformation of matter and energy, chemistry plays a central and connecting role in addressing emerging polycrises faced by Earth and Societal Systems. Outside our classrooms students live in a world characterized by conflict, environmental degradation, and misinformation. And far too often, the chemistry taught in classrooms and laboratories remains compartmentalized and largely reductionistic – disconnected from those pressing global challenges.
In this talk we will introduce the work of several project teams from the International Union of Pure & Applied Chemistry, who have led the profession forward with visionary initiatives focused on systems thinking and sustainability in education and industry, to better position chemistry education, research and practice to address pressing global challenges.
We will also introduce IUPAC's recently released **Guiding Principles for Responsible Chemistry,**[1] a bold, forward-looking framework to ensure that chemistry is taught, practiced, and recognized globally as a responsible and trustworthy endeavour. The Guiding Principles were created over a two-year period by a task force of the IUPAC Committee on Ethics, Diversity, Equity, and Inclusion, and were launched in July 2025 at the World Chemistry Congress in Malaysia. The eight IUPAC Guiding Principles are positioned as an important compass to build on, complement, and significantly advance established frameworks (e.g., green chemistry, professional ethics, chemical security) and are intended to support rigorous, transparent practice amid data- and AI-driven discovery. As a global chemistry community, might we make use of these initiatives to catalyze a paradigm shift from focusing on what chemistry can do, to what chemists should do to practice chemistry responsibly for society?[2]

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Fig. 1: IUPAC's Guiding Principles for Responsible Chemistry

RC - D1 - I02
Social responsibility of chemists: A historical perspective

Ernst Homburg
Maastricht University, The Netherlands

During the last two decades the social responsibility of scientists has become an important topic, both within government policy and within the classroom. In 2013, for instance, an Expert Group within the European Union published the report Options for Strengthening Responsible Research and Innovation. And for chemistry students at universities, in 2021 a handbook was published, edited by Joachim Schummer and Tom Børsen, with the title Ethics of Chemistry: From Poison Gas to Climate Engineering. In that handbook an exposition of basic philosophical and ethical concepts is combined with discussion of historical examples, such as Poison Gas, Thalidomide, DDT, Bhopal, CO2 and climate change, Bisphenol-A, and many others. In my lecture, I will use examples such as these from a different angle. The central theme of the talk is how the concept ‘Social Responsibility’ evolved over time within the chemical community. Starting with the professionalization of chemistry in the nineteenth century, I will follow the chemists in society, that started working for instance in industry and in the military, united themselves in chemical societies, and worked in research institutes and regulatory bodies of government. How did these chemists and chemical communities react to major incidents such as the use of poison gas and the atomic bomb, the world-wide pollution by pesticides, etc., etc.? But also: what were their dreams about the role that chemistry should play in society? Because social responsibility is not only about what chemists should not do, but also about what they should do. Next to that, I will look in particular to the role that the distinctions between pure and applied chemistry played in those debates, as well as to how chemists, industry, and governments responded to the distinction between foreseen and unforeseen consequences.

RC - D2 - I01
Chemistry at the crossroads: Building knowledge between collections and communities

Federica Pozzi
Centro per la Conservazione ed il Restauro dei Beni Culturali "La Venaria Reale", Italy

Chemistry plays a key role in the study, preservation, and valorization of cultural heritage, providing tools to investigate materials and techniques, inform conservation strategies, and drive a wide range of activities, including advanced training and education, dissemination to specialized audiences, and public engagement. Experiences across different institutional contexts—from museums to conservation centers—highlight the diverse ways in which chemical expertise not only contributes to the increasingly complex field of heritage science, but also enhances its role in serving and engaging society.
At the CCR "La Venaria Reale", chemistry is embedded within a broader societal mission. Beyond supporting conservation treatments and scholarship in archaeology and art history, scientific research and analysis underpin cutting-edge research projects in collaboration with institutions worldwide and contribute to international cooperation programs in emerging countries. In addition to hosting the University of Turin's Master's Degree in Conservation and Restoration of Cultural Heritage, the Center places strong emphasis on advanced training at multiple levels, integrating chemistry into both academic and professional education through courses, seminars, and workshops for students and practitioners alike. It also organizes and participates in a broad array of outreach initiatives aimed at schools and the general public.
Interdisciplinary collaboration and sustainability are central to all activities, while ethical considerations—including cultural sensitivity and inclusivity, transparency and accountability, equitable access to knowledge, long-term stewardship, and responsible community engagement—guide decision-making and best practices. In this context, chemical expertise serves as a vehicle to support heritage management, foster capacity building, and generate socially impactful outcomes that connect science, culture, and society. This keynote lecture explores the multifaceted role of chemistry for cultural heritage, highlighting the balance between in-depth collections-based research and broader societal service, and offering insights into the responsibilities, challenges, and opportunities for chemists working at the intersection of science, conservation, and communities.

RC - D4 - I01
Beyond the black box: Human understanding and ethical limits of AI for chemistry

José Ferraz-Caetano
HOLOSS Research – Centre for advanced science, technology and public value –Monção, Viana de Castelo, Portugal; LAQV-REQUIMTE, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Porto, Portugal

As artificial-intelligence (AI) becomes embedded in chemical research, the central question is no longer, "what AI can do for chemistry", but "what it is doing to chemistry" (Figure1). AI for chemistry now ranges from simple tools that help with literature searches to complex systems that suggest mechanisms, syntheses, and design experiments with little human input. In this increasingly technical landscape, AI-driven analysis can conceal many ethical stakes, making the implications of its use invisible to experts and the public. I will argue that this opacity lets technical success sideline ethical reflection.
A central theme will be, what counts as understanding a phenomenon? When predictions from "black-boxed" models systematically outperform transparent methods, it becomes tempting to compare accurate prediction with genuine understanding[1]. Yet, scientific understanding is not exhausted by correct outputs. It involves human movements of thought and feeling, which form concepts for responsible courses of action. These integrative capacities cannot be handed over to a machine. I argue that reliance on such "intelligent intelligences" may subtly recast the chemist from discoverer, into a curator of opaque intelligences.
Finally, I will address three pressing consequences. First, the risk of fraudulent use of AI in chemistry, amplified by the difficulty of scrutinizing algorithmic explainability[2]. Second, the crowding-out of older techniques, as optimized AI pipelines suppress methodological diversity, making the field vulnerable to bias and error. Third, the conceptual confusion when we assign "thinking" or "innovation" to AI. What is a machine doing when it "learns" and where must human decision-making take over? The talk concludes by outlining a governance method between chemistry and the humanities, treating AI not as a tool, but as a new epistemic agent whose integration must be deliberately shaped.

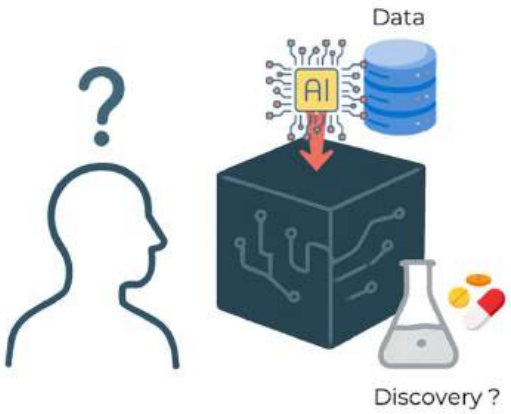

Fig. 1: How can chemists explain an opaque AI "black box" that generates chemical predictions?

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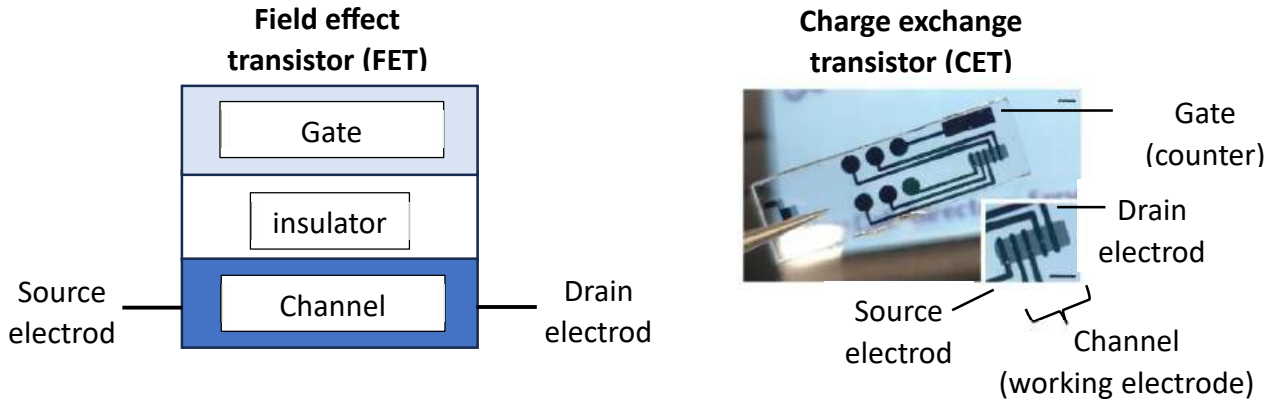
Perspectives in Analytical & Physical Chemistry (APC)

APC - D1 - O01
Charge exchange transistor: An extension of electrochemistry

Xiaoyang Chen[1], Al-Amin Dhirani[1,2]
[1]Dept. of Physics, University of Toronto, Canada; [2]Dept. of Chemistry, University of Toronto, Canada

Modern computing has at its heart the field effect transistor (FET) - an elegant 3-electrode device that enables switching – see figure. Application of a gate voltage classically charges the channel and switches its resistance. Here, we present charge exchange transistors (CETs) that combine FET with electrochemistry – see figure. We use a thin metal film as the working electrode (CET channel) and monitor its resistance during cyclic voltammetry. The metal film exhibits remarkable resistance peaks during metallocene - metal film redox charge exchange. Multiple evidence, including various types of measurements, kinetic modelling and density functional theory calculations are consistent with a multi-step redox pathway that includes the formation/destruction of a hybrid metallocene + metal state. These results provide important new insight into mechanisms involved in charge exchange; conversely, they point to an important application of CET as a means for probing and potentially exploiting such phenomena.



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APC - D1 - O02
Electrochemical confinement as a tool for nanoscale fabrication and redox control

Noah Al-Shamery[1,2], Rafael A. Vicente[1,3], Bethanie Dean[1,4], Dimitrios Valavanis[1], Jonas Lorenz[5], Stanislav K. Petrovskii[5], Pooi See Lee[2], Paul Wilson[1], Patrick R. Unwin[1,6], Kirill Monakhov[1,5,7]
[1]University of Warwick, UK; [2]Nanyang Technological University, Singapore; [3]UNICAMP, Brazil; [4]Analytical Science CDT Warwick, UK; [5]Leibniz Institute of Surface Engineering (IOM), Germany; [6]Hartnoll Centre for Experimental Fuel Technologies Warwick, UK; [7]Institute of Advanced Study Warwick, UK

Understanding and controlling electrochemical processes at small length scales is essential for the development of functional materials and molecular systems. Scanning electrochemical cell microscopy (SECCM) is a scanning probe technique in which a micro- to nanoscale electrolyte meniscus is brought into contact with a surface, enabling localized electrochemical measurements, deposition, and surface modification.[1]
Here, we show how electrochemical confinement provided by SECCM can be used for both localized fabrication and the interrogation of redox-active molecular systems, illustrated through two complementary case studies. First, we address a general challenge in polymer micro- and nanofabrication: reliable chemical characterization of deposits formed below the far-field optical diffraction limit. By combining SECCM with scattering-type scanning near-field optical microscopy and nanoscale infrared spectroscopy, we achieve chemically resolved mapping of electropolymerized polyaniline and polypyrrole structures with sub-50 nm spatial resolution. This approach reveals electrolyte-dependent growth behavior, nanoscale heterogeneity, and embedded inorganic phases that are inaccessible using conventional electron or far-field spectroscopic techniques.[2]
Second, SECCM is used to investigate the redox behavior of carboxyl-functionalized vanadium(V/IV)-based polyoxometalates (POMs) under well-defined local electrochemical conditions.[3] Localized measurements reveal redox heterogeneity arising from variations in the interfacial chemical environment of the POMs that are averaged out in bulk electrochemistry. Spatially defined deposition combined with localized electrochemical readout enables reversible redox write-read cycles, while density functional theory links the observed behavior to hydrogen-bond-mediated electronic effects within the molecular framework.
Together, these results demonstrate how electrochemical confinement, combined with nanoscale characterization, enables new approaches to fabricating and programming functional materials and redox-active molecular systems.

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APC - D1 - O04
Interfacial effects in indium(III) ion electroreduction

Alicja Pawlak[1], Agnieszka Nosal-Wiercińska[1]
[1]Dept. of Analytical Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Sklodowska University, Poland

Indium is a metal of key importance for modern electronic technologies. According to data reported by the United States Geological Survey (USGS), the largest share of global indium consumption is associated with the production of indium tin oxide (ITO), whose thin films serve as transparent conductors in, among others, LCD displays and various optoelectronic applications [1-2]. Despite intensive research efforts aimed at developing alternative materials, ITO continues to dominate this class of practical applications [3]. This situation justifies the need for in-depth fundamental studies on the behaviour of In(III) ions in environments relevant to electrochemical processes.

In this work, the influence of supporting electrolyte composition on the electroreduction of indium(III) ions in mixed aqueous–organic systems was investigated, with particular emphasis on the role of solvent type and the effect of added organic compounds fulfilling the criteria of the cap-pair effect in controlling the kinetics and mechanism of the electrode process. The study was carried out using cyclic voltammetry (CV), square-wave voltammetry (SWV) and direct-current (DC) polarography, while electrochemical impedance spectroscopy (EIS) was applied for comparative purposes. The calculated kinetic and thermodynamic parameters were correlated with measurements of organic component adsorption at the amalgam electrode (R-AgLAFE)/solution interface, allowing the observed kinetic changes to be related to modifications in the structure of the electrical double layer (EDL) [4-5].

The obtained results indicate that an appropriate selection of supporting electrolyte composition constitutes an effective tool for modulating the course of In(III) ion electroreduction. This knowledge may in the future provide a valuable basis for the rational design of technological processes, including those related to indium recovery or the electrodeposition of metallic thin films with tailored structure.

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APC - D1 - O05
Lipid composition influences the formation of vesicle lamellarity

Obed Obeng-Gyasi[1], Jyothsna Karman[1], Andrew Clullow[2], Evelyne Deplazes[1]
[1]School of Chemistry and Molecular Bioscience, University of Queensland, Australia; [2]Australian Nuclear Science and Technology Organisation, Australia

Vesicle lamellarity significantly influences lipid packing, fluidity, and membrane permeability, thereby affecting bilayer-molecule interactions. Although it is commonly assumed that freeze/thawed and extruded vesicles are unilamellar, some multilamellar vesicles (MLV) remain. The stacked bilayer arrangement of MLVs differs from the single-bilayer architecture of the cell's plasma membrane and thus can affect observations and translation of insights from vesicle-based assays (e.g. dye leakage or fluidity assays) to cellular systems.
In this study, we investigate the effect of lipid composition on lamellarity and bilayer structure in vesicles with simple and complex lipid compositions, specifically, anionic and zwitterionic phospholipids and sterols. Our results show vesicles containing zwitterionic phosphatidylcholine (POPC) lipids only have a low fraction of externally accessible lipid (f_{acc}), indicating a high degree of multilamellarity. Adding ergosterol, the f_{acc} further decreased, indicating that sterols significantly increase the presence of MLVs. This was accompanied by bilayer structural changes, including reduced area per lipid, increased bilayer and hydrophobic thickness, signifying an altered membrane fluidity compared to PC vesicles. The addition of phosphatidylethanolamine (POPE) caused a further reduction in facc and amplified the structural changes induced by ergosterol. Adding anionic lipid, phosphatidylserine (POPS), caused a significant increase in f_{acc} compared to POPC or POPC-ergo vesicles, without significant changes in the structural parameters.
Our results demonstrate that ergosterol and POPE significantly increase the degree of multilamellarity in vesicles, while causing bilayer structural modification, and that at least 10% of POPS is required to form predominantly unilamellar vesicles.

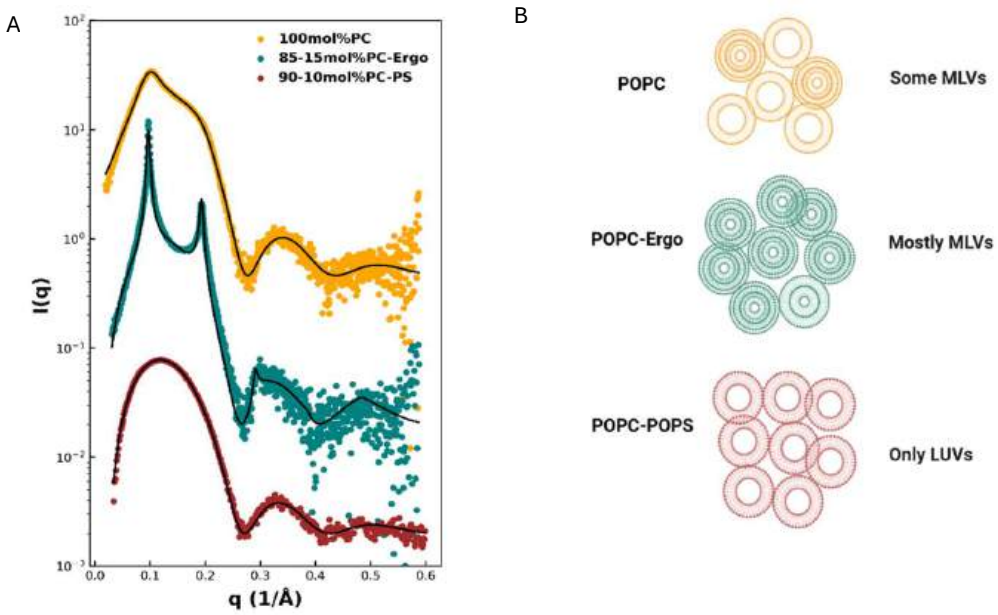

Fig. 1. A) Scattering profiles (coloured dots) and model fits (black lines), and B) lamellarity schematics for POPC, POPC–Ergo, and POPC–POPS vesicles

APC - D1 - O06

High-throughput continuous slug flow platform for investigating non-photochemical laser-induced nucleation mechanisms

Rishi Bharadwaj Morthala[1,2], Christophe Vande Velde[1], Wim Wenseleers[2]
[1]iPRACS, Universiteit Antwerpen, Belgium; [2]NANOrOPT, Universiteit Antwerpen, Belgium

Non-photochemical laser-induced nucleation (NPLIN) offers a novel pathway to non-invasively trigger crystallization in supersaturated solutions. However, the precise underlying mechanisms at play remain debated, largely due to the stochastic nature of nucleation. Conventional studies predominantly rely on batch vials and suffer from poor reproducibility, handling disturbances, and labor-intensive operations. This study introduces a continuous gas-liquid slug flow platform to overcome these limitations. Our approach eliminates manual sample handling and enables generation of large, statistically significant datasets required to unravel NPLIN mechanisms. We developed a custom flow setup where a T-mixer generates gas-liquid slug flow from undersaturated KCl solutions filtered through a 0.22 µm membrane to eliminate dust interference. Each KCl slug functions as an isolated micro-reactor requiring minimal volume compared to batch vials. Upon entering a temperature-controlled zone, the slugs achieve supersaturation (S=1.0 – 1.12) over a residence time before being irradiated by a Nd:YLF pulsed laser (7 W, 527 nm, 1 kHz, 200 ns) with adjustable peak power. Nucleation is observed post laser irradiation via a digital camera to quantify nucleation probability. Crucially, a synchronized pulse delivery mechanism is implemented which allows for precise control over number of pulses and spatial separation within each moving slug.

Validation experiments confirmed precise temperature control (±0.1 °C) and generation of stable slug flow with tunable slug length, speed and frequency. We have successfully observed laser-induced nucleation in supersaturated slugs with minimal spontaneous nucleation detected in non-irradiated control slugs. Furthermore, we confirm the absence of secondary nucleation post irradiation. Preliminary experiments indicate positive correlation between nucleation probability and laser power. Current work is focused on mapping these trends against supersaturations, polarization, pulse count. At the conference, we will present comprehensive dataset comparing nucleation probabilities across various parameters. Specifically, we will demonstrate how the spatial separation of pulses influences the nucleation rate, providing new insights into NPLIN.

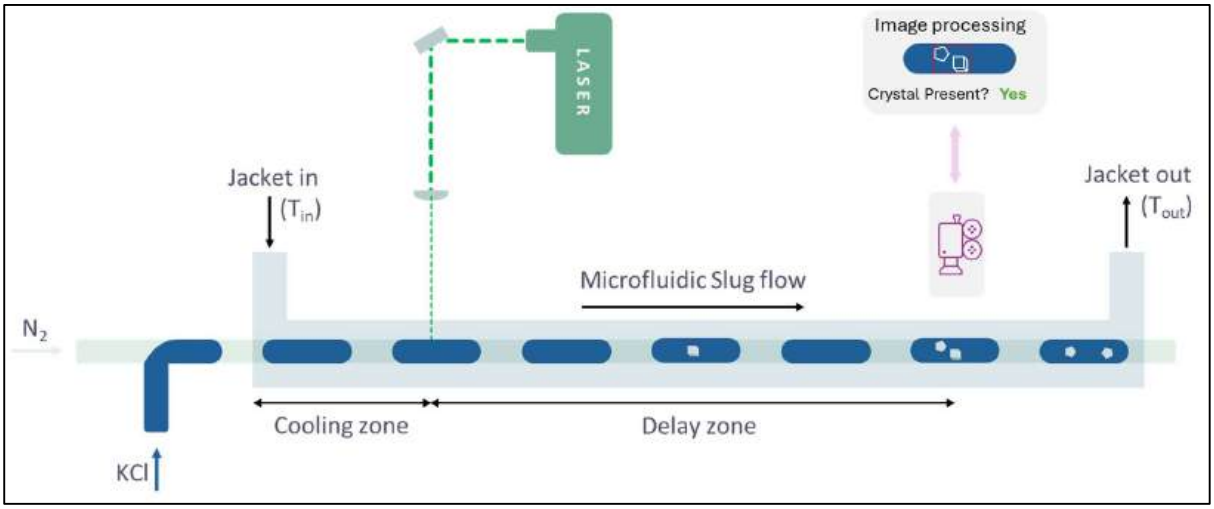

Fig. 1. Schematic representation of NPLIN setup

APC - D1 - O07

Excited-state proton transfer in Ru(II)- and Fe(II)-complexes with pyrazine-moieties – Towards iron-based photobases

Niklas Klosterhalfen[1,2], Benjamin Dietzek-Ivanšić[1,2]
[1]Leibniz Institute of Photonic Technologie, Germany; [2]Leibniz Institute of Surface Engineering, Germany

This contribution discusses novel Ru(II)- and Fe(II)-complexes with pyrazine moieties with regard to their photophysical properties.[1] The incorporation of the pyrazine moiety into the first coordination sphere of the metal centre allows for an indirect excitation of the photobasic pyrazine via metal-to-ligand charge-transfer. This approach has the potential to shift the wavelengths required to trigger photobasicity from the UV to the red part of the visible spectrum, opening the door for a variety of applications.

The concept of modifying the first coordination sphere of TMCs to include photoacidic/photobasic moieties was pioneered by the groups of Taube and Demas.[2] Since, this concept was transferred to mononuclear Re(I), Os(II), Ir(I) and Pt(II) complexes,[3] as well as to trimetallic complexes featuring Fe(II), Ru(II) and Os(II).[4] While the original design profited from the long excited-state lifetimes of Ru(II) complexes, applications with the isovalent Fe(II) counterparts are challenged by their low-lying metal-centered (MC) states, which favor nonradiative decay pathways of the initial optical excitation.[5]

The design of the complexes reported here was thus motivated by their use in excited-state proton transfer (ESPT) reactions, which can be applied, for example, to control pH-sensitive chemical reactions via illumination. By employing a combination of steady-state and transient absorption spectroscopy to study their ground- and excited-state protonation behaviour, we highlight the fast internal relaxation dynamics in the complexes. Assisted by (TD)DFT calculations we derive at structure-dynamics-function relation for the novel transition-metal-complex based photobases.[6]

Acknowledgement: This work was financially supported by the German Science Foundation within the Priority Program “Light-controlled reactivity of metal complexes” (project number 493768838).

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APC - D1 - O09

The fate of the proton in protic and aprotic ionic liquids: Acidity and ion transfer studied by Raman spectroscopy

Aurelie Rensonnet[1], Irelie Ebardo[2], Alyna Lange[2,4], Patricia Hunt[2,3], Andreas Tubert[4], Cedric Malherbe[1]
[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liège, Belgium; [2]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand; [3]Dept. of Chemistry, Imperial College London, UK; [4]Institute of Chemistry, University of Potsdam, Germany

Ionic liquids (ILs), interesting for their tunable solvation behavior and ability to reach high acidities, are commonly classified as protic (PILs) and aprotic (AILs). PILs result from proton transfer between a Brønsted acid and a Brønsted base, yielding a protonated cation. However, acidity is not restricted to PILs, as both PILs and AILs can be acidic depending on whether the proton is associated with the cation or with an acidic anion, respectively.[1] Moreover, high acidity can also be achieved by dissolving Bronsted acids in ILs, owing to the weakly coordinating nature of their anions, leading to high proton activity.

Acidity in ILs is commonly evaluated using Hammett acidity functions, based on the protonation of weakly basic indicators. Protonation is traditionally monitored by UV-Visible spectroscopy, but Raman spectroscopy has been recently implemented in AILs, which allowed us to reveal the influence of the indicator concentration on acidity determination, an effect previously unexplored.[2,3] These results also highlighted the presence of ion pairing in ILs, and its possible distinct impact on UV and Raman spectra, leading to differences in the measured acidity.

Raman spectroscopy is also a valuable tool for probing proton transfer in PILs. Studies were performed on a sulfonic acid-functionalised ammonium IL paired with a methanesulfonate anion in the presence of different amounts of methanesulfonic acid. The analysis of Raman specific bands of the IL, coupled with computational modeling using SMD-GIL solvation model, enabled discussing the evolution of the proton chemical environment, hydrogen bonding and cation-anion interactions in the IL upon increasing acid concentration.

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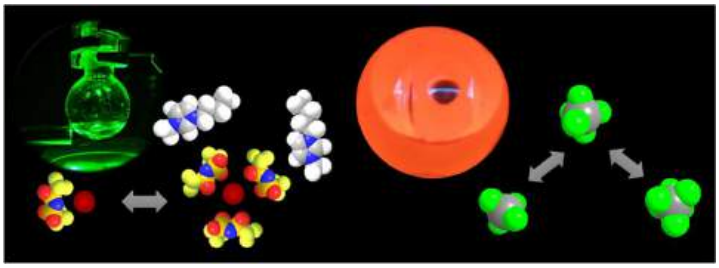
APC - D1 - O10

Raman spectroscopy for probing extreme chemical systems: From high-temperature molten salts to super-acidic room temperature ionic liquids

Cedric Malherbe[1], Aurelie Rensonnet[1], Gauthier Eppe[1]
[1]Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liege, Belgium

Extreme chemical systems such as high-temperature molten salts, supercritical fluids and super-acidic ionic liquids pose major analytical challenges due to their reactivity, optical opacity, volatility or limited sample accessibility. Over the past decade, Raman spectroscopy has emerged as a uniquely versatile tool for the in situ and non-destructive characterisation of such environments, provided that dedicated optical configurations, rigorous spectral modelling and advanced chemometric analysis are implemented to extract fundamental physico-chemical information and enable robust analytical developments. This contribution presents a methodological perspective based on Raman spectroscopic investigations of chemically extreme acidic systems, spanning temperatures from ambient conditions up to 1000 °C and encompassing two acidity regimes. In situ polarised Raman measurements performed on aluminium fluoride-based molten salts allow the identification of an unsuspected pentafluoroaluminate complex within the melt and enable the direct quantitative determination of melt composition under industrially relevant operating conditions[1,2]. More recently, the methodology has been applied to non-protic ionic liquids exhibiting super-acidic behaviour, where Raman spectroscopy enables the experimental estimation of proton solvation free energies and provides direct insight into acidity levels using Hammett acidity scales[3,4]. Beyond the specific systems investigated, this work highlights the broader potential of Raman-based methodologies for studying extreme chemical media using miniaturised instrumentation such as those developed for highly constrained environments, including space exploration.



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APC - D1 - O11
Water-driven self-assembly pathways for thermostable and adaptive supramolecular materials

Chien-Lung Wang[1]
[1]*Dept. of Chemistry, National Taiwan University, Taiwan*

Nature exploits non-covalent interactions, with water as a key mediator, to stabilize biomolecular structures and direct their functional conformations under extreme environments. Inspired by this principle, we investigated how water can guide and reinforce supramolecular assemblies in synthetic systems. Two dendritic amphiphiles were studied: a branched amphiphile forming hydrated hexagonal columnar (Col_h) phases via water-induced self-assembly (WISA), and a wedge-shaped, shape-shifting dendron (SD) undergoing rare phase transitions upon hydration. In the Col_h phase, artificial water channels (AWCs) encapsulate both bulk-like and interfacial water, whose hydrogen-bonded networks confer thermophilicity, preventing isotropization even above the boiling point of water while simultaneously accelerating water transport at elevated temperatures. For the SD system, cooling from the isotropic melt trapped molecules in a metastable Frank–Kasper σ phase with symmetry breaking. Water vapor disrupted micellar packing and unfolded cone-shaped SDs, enabling improved chain–chain ordering and inducing a σ → hydrated lamellar (L_w) transition. Encapsulated water molecules further stabilized the Lw, double-diamond quasicrystal (DDQC), and hydrated σ phases. Collectively, these findings establish water as an active structural modulator in synthetic supramolecular chemistry: it not only enhances thermal robustness and transport properties but also guides conformational ordering to unlock new phase behaviors, echoing nature's strategies for adaptive molecular organization .

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APC - D1 - O12

Evaluation of cellulose-based passive adsorbers for capturing acetic acid using HS-TD-GC–MS and Magic Chemisorbers

Chiara Biribicchi[1], Jessica Chasen[1], Laura Maccarelli[1]
[1]Conservation Center, Los Angeles County Museum of Art, USA

Cellulose acetate, a semi-synthetic plastic commonly found in museum collections, undergoes hydrolytic degradation that releases acetic acid as a byproduct, producing the characteristic vinegar odor known as “vinegar syndrome.” Once emitted, acetic acid acts as a reaction catalyst, accelerating hydrolytic deacetylation and further increasing the degradation rate of cellulose acetate objects. Reducing acetic acid concentrations in storage enclosures for cellulose acetate has therefore become an important area of focus in museums, as it can help reducing the deterioration of these objects[1].

This study evaluates the efficiency of newly developed cellulose-based passive adsorbers as a potential solution for capturing acetic acid emitted by cellulose acetate objects, using “Composition” (1938) by László Moholy-Nagy as a case study. The approach employs a new semi-quantification protocol that integrates headspace thermal desorption (HS-TD) coupled with gas chromatography–mass spectrometry (GC–MS) and the Magic Chemisorbers PEG-S[2].

To date, no studies have applied semi-quantitative methods to evaluate how acetic acid concentrations in enclosed environments containing cellulose acetate objects differ in the presence or absence of passive adsorbers. Furthermore, the use of Magic Chemisorbers for this purpose remains unexplored, as solid-phase microextraction (SPME) is typically employed for the determination and quantification of acetic acid in museum environments.

The project aims to evaluate the analytical performance and practical applicability of this method for detecting and semi-quantifying acetic acid in enclosed environments, as an easily implementable alternative to SPME. The resulting protocol will improve our understanding of how conservation strategies influence the condition of cellulose acetate and support the development of more effective, sustainable storage solutions for sensitive materials.

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APC - D1 - O13

Mass-dependent and independent isotopic fractionation in ozone – Theoretical modelling of experimental data

Peter Reinhardt[1], François Robert[2]

[1]Laboratoire de Chimie Théorique, Sorbonne Universitté and CNRS UMR7616, France; [2]Institut Origine et Évolution (O & E), Muséum National d'Histoire Naturelle et Sorbonne Université, IMPMC-UMR 7590 CNRS, France

Oxygen isotope ratios are important data for paleoclimatic studies of ice cores or other water samples, or to classify meteoritic material. Ozone exhibits an unusual and large deviation from terresterial rocks or water samples, with comparable enrichments in heavier isotopes ^{17}O and ^{18}O, presenting a physico-chemical puzzle since its discovery in 1983.

Starting from the Lindemann process of ozone production via the concurrential stabilization of decay of an activated O_3^* complex, we add an ad-hoc correction of classical-trajectory scattering simulations fully taking into account the quantum-mechanical principle of indiscernability. This correction, based on different lifetimes of symmetric (A-X-A) or asymmetric (A-X-B) three-atomic complexes, produces qualitatively the observed isotope fractionation.

For two different $O + O_2$ potential surfaces,[1,2] variations of the mass-independent fractionation is observed along the experimental trends. Coupling the mass-independent fractionation to known mass-dependent corrections[3] gives us the possibility to estimate the kinetic constant for ozone-stabilizing collisions with a third body, which in turn allows to access as well the pressure dependence of the isotope fractionation.

Again, obtained results are in qualitative agreement to published experimental data.

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APC - D1 - O14

Probing molecular alignment and microstructural heterogeneity in polymers via high-resolution polarized O-PTIR imaging

Karolina Kosowska[1], Honorata Oleś[1,2], Tomasz P. Wrobel[3]

[1]Solaris National Synchrotron Radiation Centre, Jagiellonian University, Poland; [2]Doctoral School of Exact and Natural Sciences, Jagiellonian University, Poland

In recent years, optical photothermal microscopy (O-PTIR) has been gaining popularity in biological[1] and materials research[2]. It simultaneously provides mid-infrared and Raman spectra. Because spatial resolution depends on the visible probe, it is wavelength-independent and up to several dozen times greater than FT-IR microscopy[3].

The phenomenon of IR absorption dependence on polarization angle and orientation function distribution algorithm (ODF) can be successfully used to determine the orientation of molecules in 3D space (Figure 1)[4-6]. Using O-PTIR microscopy, we have obtained information on molecular organization in a semi-crystalline polymer with submicron resolution[5], entering a field dominated by X-ray methods. We investigated the effect of plasticizers and nano-nucleators on the molecular organization in poly(L-lactic acid). The new method not only provides high resolution but is sensitive to subtle changes in morphological organization, such as changes in lamella angle in space (Figure 2).

This research was supported by the National Science Centre, Poland (SONATINA 7, “Study of the effect of modifiers on the crystallization process of thermoplastic polymers: polarized IR microscopy below the diffraction limit”, Grant No. 2023/48/C/ST4/00176). O-PTIR measurements were performed at the CIRI beamline under the provision of the Polish Ministry and Higher Education project Support with the use of research infrastructure of the NCPS SOLARIS under contract nr 1/SOL/2021/2.

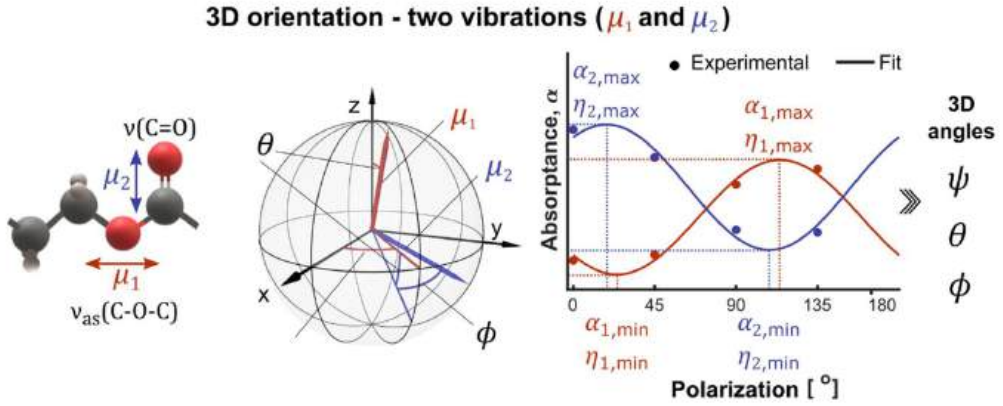

Fig. 1. Visualization of the determination of the 3D orientation of molecules with used of of two perpendicular transition dipoles μ_1 and μ_2. Based on[5].

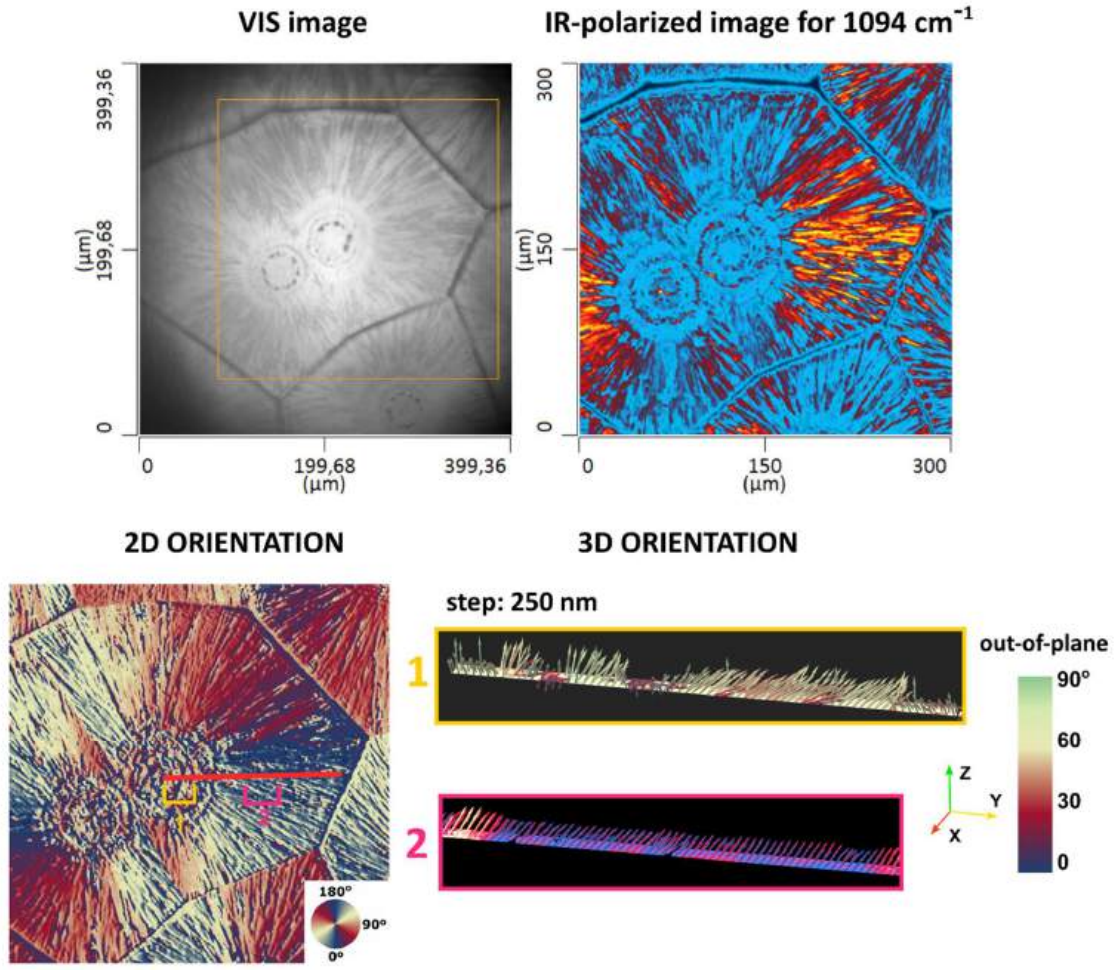

Figure 2. O-PTIR measurement of poly(L-lactic)-based sample after crystallization in non-isothermal conditions: VIS image, IR-polarized image for 1094 cm^{-1}, map of in-plane orientation of molecules, and 3D orientation of molecules along red line limited to region 1 and 2.

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APC - D1 - F01

The development of an analytical method for assessing the cornea-on-chip as a predictive *in vitro* model for ocular drug absorption

Evelyne De Vos[1,2], Debbie Le Blon[1], Tim Boogaerts[2,*], Carina Koppen[1,*]
[1]Antwerp Research Group for Ocular Science, University of Antwerp, Belgium; [2]Toxicologicial Centre, University of Antwerp, Belgium
** joint senior authorship*

The cornea-on-chip[1] is a microfluidic model that replicates the human corneal barrier, offering a promising alternative to animal testing for ophthalmic drug development. To validate its permeability characteristics, comparison with the *ex vivo* human cornea is essential. This study aims to develop, optimize and validate a robust liquid chromatography-tandem mass spectrometry (LC-MS/MS) method to quantify a selection of chemical compounds with different physicochemical properties, including carbamylcholine, acetazolamide, metformin, hydrochlorothiazide, serotonin, doxylamine, minoxidil and amitriptyline. This method will be used to compare drug permeation across the cornea-on-chip and the *ex vivo* human cornea. The analytes span a wide LogP range (−3.14 to 4.37) and molecular weights (129.10 to 296.96 Da), to assess the model's ability to differentiate between highly, moderately, and poorly permeable drugs. A sensitive LC-MS/MS method was developed to quantify these compounds at low concentrations. Multiple chromatographic columns were evaluated, including Atlantis T3, Biphenyl, Trinity and iHILIC-fusion. The latter was selected for its ability to achieve effective separation of both polar and apolar compounds. A high-throughput sample preparation method was developed based on protein precipitation and centrifugal filtration for sample clean-up. The optimized LC-MS/MS method successfully quantified all compounds within a 2 µL sample volume, a critical requirement for cornea-on-chip analysis. Preliminary experiments confirmed that sample dilution did not comprise method sensitivity and improved matrix effects. This robust method was validated in accordance with ICH M10 guidelines, ultimately supporting the cornea-on-chip as a reliable alternative to animal testing. The method demonstrated strong performance across key validation parameters: accuracy, precision, linearity, carry-over, matrix effects, and both absolute and relative recovery. A multi-level calibration curve was used for compound quantification with a linear range from 1.5 mM to 0.002 mM. Internal standards compensated for matrix effects across multiple matrix compositions, including Krebs buffer, and both epithelial and endothelial cell culture medium.

This work is made possible through funding from the Fonds voor Wetenschappelijk Onderzoek-Vlaanderen (FWO, project number: 1SG3325N). The research was conducted under the supervision and guidance of Dr. Tim Boogaerts (postdoctoral researcher, Toxicological Centre). The work was performed within the Toxicological Centre, led by Prof. dr. Adrian Covaci and Prof. dr. Alexander van Nuijs.

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[1] The cornea-on-chip (CoC) is a microfluidic device designed as a microscopy slide, that incorporates eight tissue-engineered corneal constructs comprising of all cellular layers of the human cornea. This provides a physiologically relevant *in vitro* model for evaluating novel ophthalmic formulations during preclinical development.

APC - D1 - F02
Emulsifying properties of cetearyl olivate and sorbitan olivate in semi-solid cosmetic matrices

Marta Marzec[1], Iga Ledzińska[1], Izabela Nowak[1]
[1]Adam Mickiewicz University, Poznań, Faculty of Chemistry, Dept. of Applied Chemistry, Poland

Cetearyl olivate and sorbitan olivate are non-ionic emulsifying agents derived from olive oil fatty acids, widely used in cosmetic formulations due to their favorable physicochemical properties and natural origin. The present study focuses on the development and characterization of semi-solid cosmetic systems in the form of oil-in-water (O/W) emulsions intended for hand care applications, formulated using a natural emulsifier system Olivem® 1000 (based on cetearyl olivate and sorbitan olivate). Selected vegetable oils, namely jojoba oil, raspberry seed oil, and sweet almond oil, were incorporated as the lipid phase to enhance emollient properties and skin compatibility.[1] The formulations were characterised in terms of physicochemistry (pH, viscosity). A long-term stability study was also carried out using the multiple light scattering method (MLS, Turbiscan®) to identify instabilities invisible to the human eye, related to both particle migration (creaming, sedimentation) and particle size changes (flocculation, coalescence). Stability assessments were carried out to ensure that the products tested behaved correctly over their declared shelf life, under specified storage conditions, and during their normal use in the final packaging.[2] After an assumed three months, a normal pH value was recorded for the formulations obtained, as well as slight changes in their viscosity over time and under the influence of the specified storage temperature. The stability of the tested cosmetic formulations was determined independently of storage time and temperature, and the type of vegetable oil used (ΔBS<3%), except for samples stored at 45 °C, for which more pronounced changes were observed. Based on the results obtained, the developed hand care products were determined to be stable for the introduction of additional active substances and qualified for the following in the next stage of application tests.

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APC - D1 - F04
Submicron-scale investigation of molecular organisation in polymers and biological tissues

Honorata Oleś[1,2], Karolina Kosowska[1], Szymon Tott[1], Tomasz P. Wróbel[1]
[1]SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Poland; [2]Jagiellonian University, Doctoral School of Exact and Natural Sciences, Poland

Optical photothermal infrared spectroscopy (O-PTIR) is an evolving vibrational technique that overcomes the spatial resolution limitations of conventional infrared microscopy due to diffraction by using a visible probe beam. The independence of spatial resolution from infrared wavelength enables submicrometre scale chemical imaging while maintaining molecular specificity. To further expand the capabilities of this approach, fluorescence-detected PTIR spectroscopy (FL-PTIR) can be employed. In FL-PTIR spectroscopy, infrared absorption is detected indirectly through photothermally induced changes in fluorescence quantum yield. Changes in fluorescence intensity, recorded with a wide-field imaging detector, reproduce the spatial distribution of infrared absorption and enable hyperspectral data acquisition in selected areas of the sample.[1] Crucially, this detection scheme is particularly suitable for autofluorescent biological tissues, eliminating the need for external labelling. In addition to high-resolution chemical imaging, quantitative information about molecular orientation can be obtained using the extended four-polarisation (4P) approach as an innovative strategy. It enables quantitative analysis of macromolecular orientation by measuring polarisation-dependent vibrational responses. In this work, we demonstrate the application of 4P analysis to both polymeric materials and biological tissues. Measurements of characteristic vibration bands enable the reconstruction of detailed two- and three-dimensional orientation maps. For polymer films, this method allows differentiation between crystalline and amorphous domains as well as the analysis of their spatially heterogeneous orientation distribution. In biological tissues, the same approach provides insight into the organisation of collagen fibres and the structural anisotropy of the tissue matrix.[2,3] By combining photothermal vibrational spectroscopy with polarisation analysis, the proposed approach provides chemically specific, high-resolution structural information. This methodology strengthens the links between analytical spectroscopy and the physicochemistry of anisotropic systems, offering new opportunities to study the relationship between structure and function in advanced materials and biomedical research.

Acknowledgement: This research was supported by the National Science Centre, Poland (SONATINA 7, “Study of the effect of modifiers on the crystallization process of thermoplastic polymers: polarized IR microscopy below the diffraction limit”, Grant. No. 2023/48/C/ST4/00176). Measurements were performed at CIRI beamline under the provision of the Polish Ministry and Higher Education project Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS under contract nr 1/SOL/2021/2.

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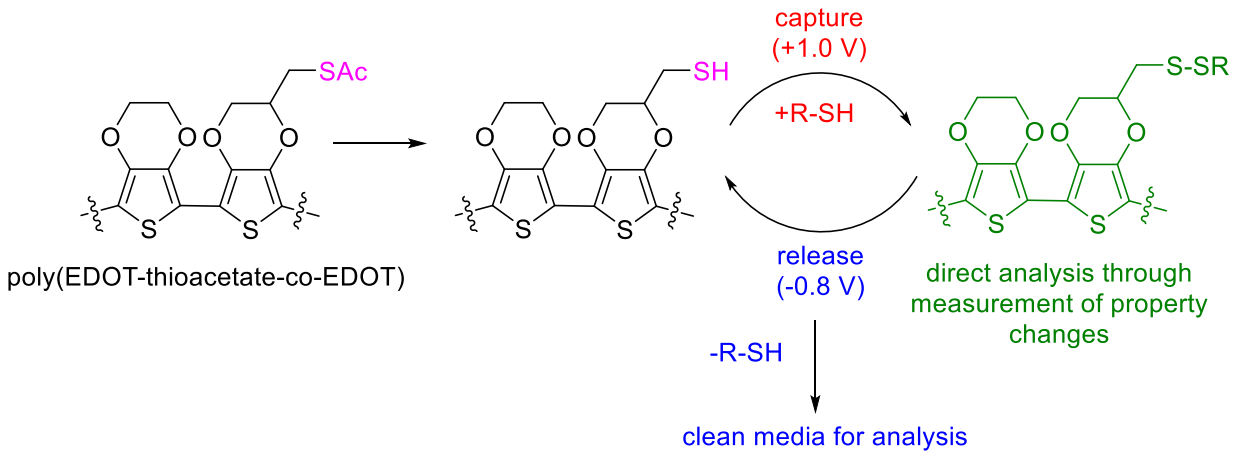
APC - D2 - O01
Sensing and capture/release of biological analytes in complex matrices

Lisa I. Pilkington[1,2], Devon T. Bryant[1,2,3], Alireza Akbarinejad[1,3], Selina Patel[4], Bicheng Zhu[1,3], Annabel Whibley[5], Craig D. Millar[4], Jadranka Travas-Sejdic[1,3]
[1]School of Chemical Sciences, University of Auckland, New Zealand; [2]Te Pūnaha Matatini, New Zealand; [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand; [4]School of Biological Sciences, University of Auckland, New Zealand; [5]Bragato Research Institute, New Zealand

Strategies that enable the sensitive and accurate analysis of chemical and biological entities are of great importance. This includes direct analysis of these analytes in complex matrices, as well as selective and controllable capture/release strategies that remove analytes of interest from other components and release into clean media for subsequent analysis. Such analytes are intrinsically linked to biological functions and their accurate analysis is a critical strategy for monitoring health and diseases. Herein we present the development of a novel platform capable of sensing and capture/release of biological entities.
This platform uses a thiol-functionalised conducting polymer, poly(EDOT-thioacetate-*co*-EDOT). The detection principle is based on conversion of the thioacetate moieties to thiols (pink) which can selectively form disulfide bonds with thiols present in a mixture *via* electrochemical oxidation (red, Figure). Changes in the properties of the polymer can be related to the concentration of analyte detected (green), allowing sensitive and selective direct detection of biological thiols such as glutathione.[1]
Alternatively, application of a reductive potential will allow the release of captured entity (R-SH) which can then be analysed using established methods (blue). Such a strategy has been applied to the analysis of cancer cells in large volumes (i.e. circulating tumour cells) and extracellular vesicles related to specific cancer cells, both with applications in cancer diagnosis, and placental extracellular vesicles for pregnancy health monitoring. Furthermore, this strategy is being adapted to the selective capture of eDNA of interest from complex samples. Details of the development and application of this first-in-class analytical sensing platform for the rapid, selective and sensitive detection of a range of important biological analytes will be presented.



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APC - D2 - O02

MAIGRET: A CRISPR-based immunoassay that employs antibody-induced cell-free transcription of CRISPR guide RNA strands

Francesca Miceli[1], Sara Bracaglia[1], Daniela Sorrentino[1,2], Alessandro Porchetta[1,3], Simona Ranallo[1,3], Francesco Ricci[1,3]

[1]University of Rome Tor Vergata, Italy; [2] University of California Los Angeles, USA; [3] Istituto Nazionale Biostrutture e Biosistemi, Italy

Here we present a two-step CRISPR-based immunoassay, named MAIGRET (Molecular Assay based on antibody-Induced Guide-RNA Enzymatic Transcription)[1], which enable the sensitive and versatile detection of specific antibodies and other proteins by integrating the advantages of CRISPR-based sensing with cell-free transcription systems.

In the first step of the assay, the target antibody binds to a pair of antigen-conjugated DNA strands, inducing their co-localization and the formation of a bimolecular complex. This complex hybridizes to the single-stranded region of an inactive synthetic template that encodes the CRISPR RNA guide strand (crRNA) specific to the Cas12a enzyme. Only upon formation of this complex the synthetic template is activated, allowing the cell-free transcription of the crRNA strand. In the second step, an aliquot of the first reaction is transferred into a mixture containing Cas12a, its double-stranded DNA activator, and a DNA hairpin reporter labeled with a fluorophore-quencher pair. The crRNA produced in the first step activates Cas12a, triggering its collateral cleavage activity and resulting in the reporter cleavage and a measurable fluorescence signal.

MAIGRET achieves highly sensitive (detection limits in the low picomolar range), specific (no signal in the presence of non-target antibodies), and selective (effective even in complex samples such as 50% blood serum) detection of target proteins. Thanks to its programmable design, the platform can be tailored for different targets, either in direct or competitive assay formats, and supports multiplexed detection using orthogonal CRISPR enzymes (e.g., Cas13), each coupled with a distinct, antibody-responsive transcriptional template. Considering the versatility of MAIGRET, we are currently developing an adaptation with a colorimetric readout by employing the collateral cleavage of a horseradish peroxidase (HRP)-DNA strand anchored on the magnetic beads as reporter system.

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APC - D2 - O03
Microfluidic paper-based devices for public health biomarkers monitoring

Raquel B.R. Mesquita[1], António O.S.S. Rangel[1]
[1]Universidade Católica Portuguesa, CBQF – Centro de Biotecnologia e Química Fina – Laboratório Associado, Escola Superior de Biotecnologia, Portugal

To develop rapid, disposable sensors for biomarkers assessment in biological fluids of non-invasive collection, natural waters and food samples was the driving force of the project PHsense – Design and development of disposable, user-friendly microfluidic sensors to monitor Public Health indicators in a One Health approach. The idea was to produce fast-response and accurate sensor devices to enable reliable and real-time response, using self-readable paper-based microfluidic devices (μPADs) applied to both environmental and biological samples, which is a breakthrough for understanding public health potential issues, thus enabling an efficient course of action.
One of the main goals of the World Health Organization (WHO) is that “all people have the right to have access to an adequate supply of safe drinking water”. Due to the economic situation in Portugal and the current water tariff scenario, recent studies have shown that the consumption of groundwater has been increasing by the population with the use of water from wells for domestic use. The homeowners are responsible for testing the water quality to ensure that it is safe for consumption and food preparation. This water can be contaminated by a variety of toxic substances and early detection is crucial to prevent harm to public health. The combined monitoring of biological fluids will enable to establish a potential contamination, hazard bioaccumulation and identify the contamination source.
In this context, μPADs can be the ideal approach, exploiting advantage of being used by untrained personnel, being almost equipment-free with low reagents and sample consumption. The developed devices represent a vital strategy for attaining effective monitoring and frequent analysis, enabling fast chemical/biochemical response resulting in a faster analytical decision. These new tools must be accurate and aligned with the ASSURED criteria established by WHO, namely “affordable, sensitive, specific, user-friendly, rapid and robust, equipment-free, and derivable to end-users”.

Acknowledgements: R.B.R. Mesquita thanks FCT—Fundação para a Ciência e a Tecnologia for the 2022.00962.CEECIND (https://doi.org/10.54499/2022.00962.CEECIND/CP1745/CT0006). This work was supported by the project COMPETE2030-FEDER-00824900, op. 16961, supported by FEDER fund within the thematic program Innovation and Digital transition (COMPETE 2030) through FCT; scientific collaboration from FCT project UIDB/50016/2020 is also acknowledged.

APC - D2 - O04

Flow-based automatic and miniaturized solid-phase extraction towards sample preparation and renewable sensors

Marcela A. Segundo[1], Diana R. Cunha[1], Sara R. Fernandes[1], Luisa Barreiros[1]
[1]LAQV/REQUIMTE, Faculty of Pharmacy, University of Porto, Portugal

Flow-based sample treatment, embedded in the principles of flow injection analysis, enables the precise management of solutions or suspensions within confined environments. By providing meticulous control over temporal and spatial parameters, these strategies significantly enhance reproducibility and facilitate the kinetic control of chemical processes.

This communication highlights recent developments in automated flow-based strategies designed to overcome traditional challenges in bioanalysis and pharmaceutical development, such as sorbent fouling, sample carryover, and analyte degradation. The implementation of Lab-on-Valve (LOV) devices combined with the bead injection (BI) concept is presented as a robust platform for automating solid-phase chemistry. Unlike conventional microfluidic devices, the BI-LOV approach allows for the microfluidic handling and renewal of beads, offering a high surface-to-volume ratio and real-time monitoring of solid-support phenomena. We discuss the online hyphenation of these systems with HPLC and MS detectors, addressing eluent compatibility and the assembly of immunoaffinity columns. Key applications demonstrate this versatility, including the reduction of ELISA protocol times from 2 hours to 5 minutes, and the rapid measurement of nanoparticle concentrations for quality control.[1-3]

Furthermore, the determination of drugs and endogenous compounds in complex matrices, such as plasma and urine, demonstrates the potential for handling real-world samples in a high-throughput, greener, and more efficient manner. Ultimately, these automated flow techniques represent a transformative approach to sample treatment, significantly improving accuracy and efficiency in the analysis of biopharmaceuticals and clinical samples.

Acknowledgments: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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APC - D2 - O05
Programmable gene circuit cascades for biosensing applications

V. Girola[1], V. Patrizi[1], S. Ranallo[1]
[1]Dept. of Chemical Science and Technologies, University of Rome Tor Vergata, Italy

Point-of-care tests play a pivotal role in early detection of infectious diseases and other clinical conditions, offering rapid, cost-effective, and sensitive capabilities. Thanks to their programmability, low cost of synthesis, biocompatibility, and chemical versatility, synthetic DNA and RNA used in nucleic acid nanotechnology have emerged as powerful tools for the development of DNA-based sensors[1]. More recently, synthetic biology has enabled the transition from cell-based to cell-free biosensors, expanding their applications in medical diagnostics[2]. By combining nucleic acid programmability with cell-free sensitivity, our group has developed the first cell-free biosensors for detecting clinically relevant antibodies[3]. However, these systems still fail to achieve the sensitivity required to detect low-abundance biomarkers. Here, we present an amplification strategy based on cascaded transcriptional cell-free gene circuits for ultrasensitive detection of clinically relevant antibodies. The binding of the target to DNA recognition modules activates a gene circuit that transcribes an RNA strand, which then triggers a secondary circuit encoding a light-up RNA aptamer. By binding its dye, the aptamer produces a fluorescence signal proportional to the target concentration. This mechanism enables a single recognition event to drive multiple transcription rounds, significantly increasing the sensitivity. We achieve picomolar limits of detection and high specificity, with no response to non-target antibodies. This approach underscores the potential of synthetic gene circuits for rapid, reliable, and accessible diagnostic applications.

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APC - D2 - O07
Detection of circulating therapeutic monoclonal antibodies for cancer monitoring

Ankita Sinha[1,*], Alejandro Chamorro[1], Alessandro Porchetta[1]
[1]*Dept. of Chemical Science and Technologies, University of Rome Tor Vergata, Italy*
**Email: ankitasinha11@outlook.com*

Programmed Cell Death Protein-1 (PD-1) and Programmed Cell Death Ligand-1 (PD-L1) are crucial immune checkpoint proteins responsible for regulating the immune response of human body. Cancer cells can manipulate this system allowing the binding of PD-1 to its ligand PD-L1 and thus activating an inhibitory signal. This results in decreased T-cell activity and anti-tumor immunity promoting tumor growth. Therapies targeting to block this PD-1/ PD-L1 pathway have transformed cancer treatment with the use of anti PD-1/PD-L1 monoclonal antibodies (mAbs) as immune checkpoint inhibitors (ICIs). The selective binding of anti PD-1 mAbs to PD-1 receptor present in active T-cells and anti PD-L1 Abs to PD-L1 in tumor cells blocks the PD-1/PD-L1 interaction and proved to be a powerful therapeutic tool to monitor prognosis of cancer patients. To detect the ICI mAbs in patients' blood samples, we propose anti PD-1 mAbs as prognostic biomarkers which can be quantified using bioanalytical techniques.

Acknowledgement: This project has received funding from the European Union's Horizon Europe Programme under Marie Skłodowska-Curie Actions (MSCA) with the grant agreement ID 101153162.

APC - D2 - O08
Activity based (bio)sensor for the monitoring of MutyH DNA glicosylase activity

Erica Belforte[1], Andrea Celeste Di Pede[1], Alessandro Porchetta[1]
[1]*University of Rome "Tor Vergata", Italy*

DNA is continuously exposed to mutagens that can induce structural damage, with significant consequences for human health. The most common oxidative lesions is 8-oxo-7,8-dihydroguanine, often resulting in G:C to T:A transversion mutations.[1] When this oxidized base pairs with cytosine within the DNA double helix, it is recognized and excised by the DNA glycosylase OGG1, initiating the base excision repair (BER) pathway. If OGG1 fails or if the damage occurs during DNA replication, a mispairing of 8-oxo-guanine:A arises. This mispairing is recognized by the glycosylase MUTYH, which removes the adenine to prevent mutagenesis. Germline mutations in MUTYH cause MUTYH-associated polyposis (MAP), a hereditary cancer syndrome that significantly increases the risk of colorectal cancer and other type of cancer.
Different molecular methods for assessing DNA repair activity have been developed so far, primarily centred on the use of indirect techniques.[2] However, they present limitations, including long analysis times and limited applicability in clinical settings. To enable direct monitoring of MUTYH activity, only few examples using chemically modified DNA probes with fluorescence readout have been reported.[3] They exhibit limited sensitivity and involve a high degree of chemical synthesis complexity.
Here, we report a DNA-based activity sensor that enables direct and sensitive monitoring of MUTYH glycosylase activity. The probe consists of a double stem–loop DNA architecture incorporating a single 8-oxoG:A mismatch and is designed to undergo a defined conformational rearrangement upon MUTYH-mediated base excision repair. This structural transition results in fluorescence signal activation, allowing real-time monitoring of MUTYH activity. The platform was validated using purified enzymes and biological samples, demonstrating its potential as a versatile tool for studying MUTYH function in complex matrix.

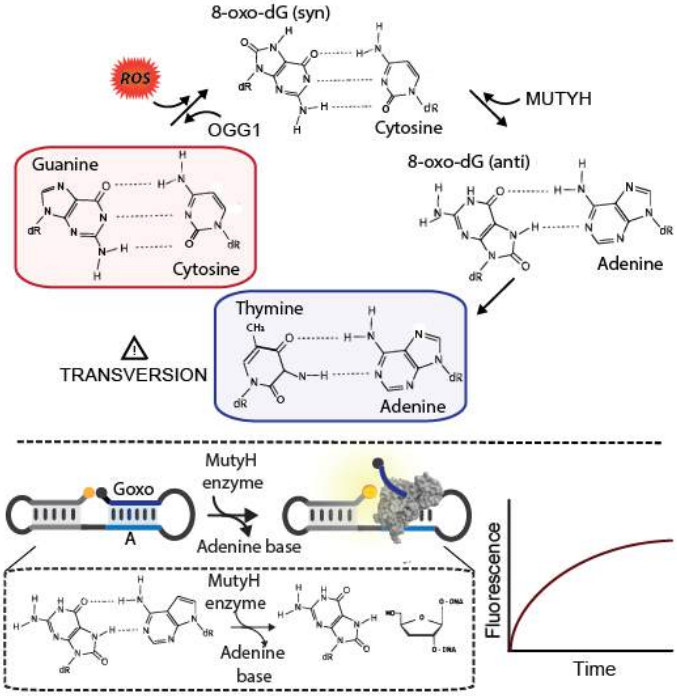

Fig. 1. Schematic representation of the BER repair process and the DNA probe for the detection of MUTYH activity

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APC - D2 - 009

Integrating LC–MS and MALDI-2 MS imaging to map brain region specific distribution of endocannabinoids and their congeners

Emanuela Salviati[1], Oumaima Azeggouar wallen[2], Roberta Verde[3], Nicolas Flamand[2], Vincenzo Di Marzo[2,3], Pietro Campiglia[1], Eduardo M. Sommella[1], Fabiana Piscitelli[*3,4]

[1]Dept. of pharmacy, University of Salerno, Italy; [2]Institut Universitaire de Cardiologie et de Pneumologie de Québec and Institut sur la Nutrition et les Aliments Fonctionnels, Université Laval, Canada; [3]Institute of Biomolecular Chemistry, National Research Council of Italy, Italy; [4]Division of Mass Spectrometry, Italian Chemical Society (DSM-SCI), Italy

Endocannabinoids (eCBs) are key neuromodulators whose biosynthesis, degradation, and regional distribution critically regulate brain physiology and pathology. Accurate quantification of these lipids, together with spatial information, is therefore essential to fully understand their signaling in the brain. While targeted LC–MS lipidomics remains the gold standard for quantification, emerging mass spectrometry imaging (MSI) platforms, such as MALDI-2, offer the unique advantage of spatially resolved molecular mapping but require validation for quantitative reliability and reproducibility. In this study, we compared classical targeted LC–MS methodologies with the recently developed MALDI-2 MSI approach to compare quantification data.

Mouse brains were bisected, with one hemisphere analyzed by targeted LC–MS following region-specific extraction (hippocampus, prefrontal cortex and cerebellum) and isotope dilution, and the other by MALDI-2 MSI using a sprayed multiclass internal standard mixture to enable quantitative imaging of the same regions.

The comparison between the two approaches revealed a strong correlation in distribution of the mediators analyzed. As a representative example, 2-arachidonoylglycerol (2-AG), detected as the same molecular ion ($[M+H]^+$) in both platforms, showed substantially higher abundance in the cerebellum than in the cortex and hippocampus, with minor variations in fold change depending on the normalization approach. The challenges encountered when comparing quantification data and possible solutions will be presented. Our results demonstrate the potential of MALDI-2 to provide spatially resolved and quantitatively reliable data, supporting its application as a complementary platform to established LC–MS techniques for eCB research. Moreover, this work provides an avenue to precisely determine the endocannabinoidome across brain regions.

We acknowledge CERIC-ERIC for access to experimental facilities at University of Salerno (project n. 20247017).

APC - D2 - O10
Analytical science as a catalyst for process efficiency: The Abrocitinib 2G experience

Chris Nottingham[1], Ramu Akula[1], Alka Choudhary[1]
[1]Pfizer Process Development Centre, Global Technology, Engineering and Launch, Ringaskiddy, Ireland

The Abro 2G programme demonstrates a rigorous analytical strategy enabling the transition from proof-of-concept to regulatory submission for a streamlined two-step API manufacturing process—reducing complexity from the original four-step route. Led by Pfizer teams in Cork, Singapore, and Chennai, with CRO support, this global effort highlights the central role of analytical science in driving process innovation, cost efficiency, sustainability, and regulatory compliance.
A tailored suite of methods was developed and validated to meet the unique challenges of the new synthetic pathway. Innovations included HPLC-UV for real-time hydrogenation monitoring with automated sampling, CAD for final API characterisation, and QqQ MRM methods for pGTI testing. These were complemented by mid-IR spectroscopy for kinetic profiling, HRMS, and NMR for structural elucidation.
Initial method development at the Process Development Centre (Cork) ensured fitness-for-purpose during non-GMP phases. Subsequent GMP validation at Pfizer Chennai and transfer to Tuas (Singapore) established a globally aligned framework. The toolkit enabled rapid decision-making during kilo-lab scale-ups, including 24/7 IPC support, and ensured product quality equivalence to the first-generation API.
This case study illustrates how integrated analytical innovation and cross-site collaboration can de-risk scale-up, accelerate timelines, and deliver a robust, sustainable API route.

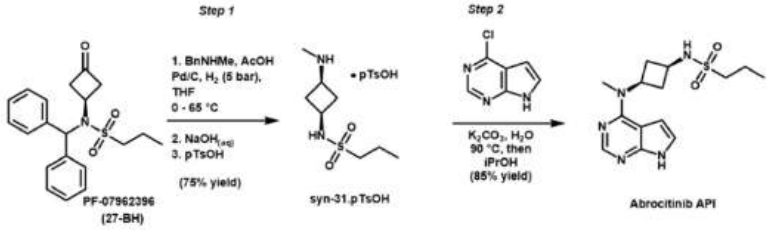

Fig. 1. 2nd Generation route to Abrocitinib

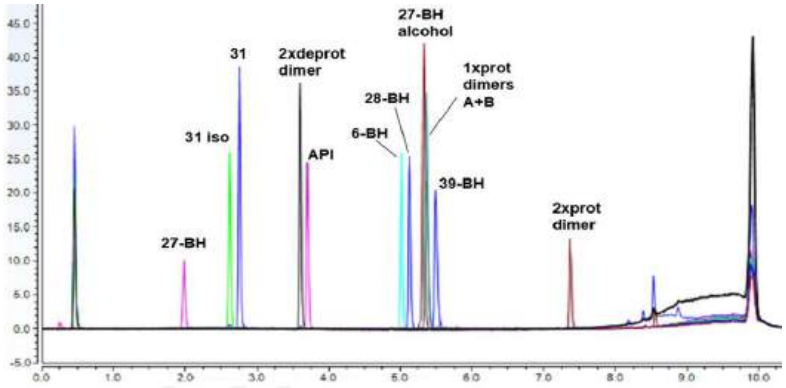

Fig. 2. Initial CAD seperation for isolated intermediste syn-31 release testing

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APC - D2 - O11
Investigation of the applicability of dimethyl carbonate as a green solvent in liquid chromatography

Rebecca Gibkes[1], Gert Desmet[1], Ken Broeckhoven[1]
[1]Vrije Universiteit Brussel, Dept. of Chemical Engineering, Belgium

High-performance liquid chromatography (HPLC) is one of the most widely used analytical techniques for the identification and quantification of components in complex mixtures. Despite its vital role in areas such as pharmaceutical analysis, environmental monitoring, food safety, and forensics, HPLC methods have a substantial environmental impact, with an estimated annual global solvent consumption of approximately 150,000 metric tons. Most LC modes, such as reversed-phase liquid chromatography, make use of water, as well as organic co-solvents to modulate analyte retention during gradient elution. One of the most frequently used co-solvents is acetonitrile, which poses significant environmental and health concerns.
To reduce the environmental impact of HPLC, several strategies have been proposed, such as the use of narrow-bore or capillary columns and the replacement of conventional organic modifiers with greener alternatives. In recent years, ethanol was the primary choice of green co-solvent due to its low toxicity, biodegradability, and potential for production from renewable resources. However, its relatively high viscosity, leads to reduced separation performance, increased back pressures, and consequently limits the achievable analysis speed.
Recently, dimethyl carbonate (DMC) has emerged as a potential alternative co-solvent due to its relatively low viscosity, green character, and high elution strength. Nevertheless, its limited miscibility with water restricts its direct application in LC. A possible solution to this is the use of mixtures of DMC with organic solvents to improve water miscibility while enabling fast and greener separation methods. Therefore, this study investigates the possibilities and limitations of using DMC as a greener co-solvent for LC by examining the miscibility of ternary mixtures of water, DMC, and different organic co-solvents. In addition, their viscosities and elution strengths are evaluated to quantify the potential reduction in solvent consumption, the effect on kinetic separation performance, and the overall improvement in method greenness.

APC - D2 - O12

Integrated analytical strategies supporting risk assessment of emerging contaminants in marine ecosystems

Alessandro Bollella[1,2], Guglielmo Pacchione[1,3], Federica Nigro Di Gregorio[1]

[1]National Centre for Water Safety (CeNSiA), Italian National Institute of Health, Italy; [2]University of Rome "Sapienza", Dept. of Environmental Biology, Italy; [3]University of Rome "Sapienza", Dept. of Chemical Science, Italy

Emerging chemical contaminants pose a challenge for environmental protection and human health, particularly in marine ecosystems where dilution coexists with long-term accumulation. Among these, per- and polyfluoroalkyl substances (PFASs) are of primary concern due to their extreme persistence, high water solubility, and resistance to degradation, promoting widespread occurrence and long-range transport.

This study aimed to develop and validate a sensitive multi-residue analytical strategy for PFAS determination in seawater, designed to integrate chemical data with ecological evaluation approaches. A solid-phase extraction–liquid chromatography–tandem mass spectrometry (SPE–UPLC–MS/MS) method was optimised for the simultaneous quantification of 30 PFASs. Water samples (500 mL) were subjected to freezing and thawing prior to extraction with Oasis WAX cartridges, followed by HPLC–MS/MS analysis. Chromatographic separation employed a dual-column setup (Accucore C18 delay column and Polar Advantage II analytical column) using a methanol–water gradient containing ammonium acetate and acetic acid, ensuring retention of both short- and long-chain PFASs while minimising background contamination.

The method demonstrated excellent analytical reproducibility, chromatographic performance, and sensitivity, with detection limits of 0.01–2.5 ng/L. A matrix-adapted limit of quantification was applied to account for background contamination in blank seawater, ensuring reliable quantification of environmental samples. The analytical performance achieved enables the generation of occurrence data suitable for integration with exposure assessment models.

Application of the validated method to Mediterranean seawater samples revealed a widespread but spatially heterogeneous distribution of PFASs. Concentrations were generally below 10 ng/L, with localised maxima up to 18 ng/L in industrialised and port-influenced areas of the Eastern Adriatic and Tyrrhenian Sea, while lower levels (≤1.7 ng/L) were observed in the Western and Southern Mediterranean. The simultaneous detection of regulated PFASs and emerging substitutes confirms the suitability of the proposed strategy for supporting PFAS risk assessment in marine ecosystems.

APC - D2 - O13

Kinetic and thermodynamic studies as a tool for understanding the adsorption mechanism of organic pollutants from aqueous media

Andrea Bogyor[1], Alexandra Ana Csavdari[1], Graziella Liana Turdean[1]
[1]Babeş-Bolyai University of Cluj-Napoca, Dept. of Chemical Engineering, Romania

Regardless of the pollution source, aqueous media can be cleansed effectively by means of adsorption. Emerging organic species in need of removal are colorants, disinfectants, and/or biocides [1-3].
Kinetic and thermodynamic studies offer insight into adsorption mechanisms. Kinetic models help establishing the nature of rate determining steps (diffusion, adsorption, combination of both), and enable determination of apparent activation energies (hinting on physi- or chemisorption). Isotherms clarify the process nature (physical or chemical), provide information about the adsorbent surface homogeneity, and determine maximum adsorption capacities. All information is necessary for effective design, optimization, and control of adsorption equipment/processes.
The adsorption of methylene blue (colorant, disinfectant) and 3,7-bis (bis (2-hydroxyethyl) amino)-phenothiazine-5-ium iodide (colorant) [4] and chlorhexidine digluconate (biocide), from aqueous solutions onto commercially available paper, is investigated here.
The advance and equilibrium state of the process are assessed at constant temperature and variable initial adsorbate/adsorbent mass ratios, by means of photometric measurements, in batch arrangements. Experimental data are analysed through the statistical model quality indicators root mean square deviation, hybrid function, and distribution of residuals [4,5]. These considered both the number of data and model parameters.
All examined species proved to follow a diffusion-driven physisorption, ruled by pseudo-second-order overall kinetics, and described by Freundlich isotherms at equilibrium.

The authors kindly acknowledge the support of the *Sapientia Hungariae Foundation* (Budapest, Hungary), *Collegium Talentum* Scholarship Program 2025-2026, and the *Transylvanian Museum Society* (Cluj-Napoca, Romania), research grant number 592.5.2/2024.

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APC - D2 - O14

Benchtop ^{19}F NMR analysis of bio-oils produced from Brewers' Spent Grains and other waste products

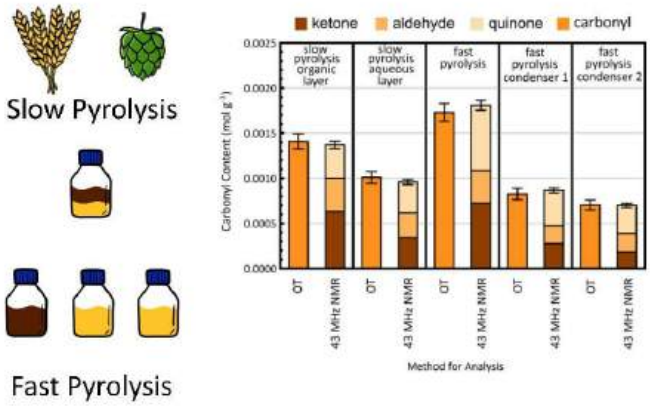
Bridget Tang[1], Katie Chong[2], Robert Evans[3,4]
[1]Aston Institute of Materials Excellence, Aston University, UK; [2]Energy & Bioproducts Research Institute, Aston University, UK; [3]Chemical Engineering and Applied Chemistry, Aston University, UK; [4]Dept. of Chemistry, University of Manchester, UK

Beer is one of the most consumed beverages worldwide and *ca*. 85 % of waste from the brewing industry is a biomass resource called Brewers' Spent Grain (BSG). Unlike biomass resources grown specifically to produce fuel, agricultural wastes such as BSG have high availability and low cost.

Pyrolysis bio-oil produced from lignocellulose biomass is a promising carbon-neutral replacement for fossil fuels. A typical bio-oil consists of hundreds of small organic molecules, including oxygen-containing compounds such as aldehydes, ketones and quinones. The quantities and identities of the oxygen-containing species are key to the long-term stability and required processing of the oil.

Nuclear Magnetic Resonance (NMR) spectroscopy is a versatile analytical tool but ^{1}H NMR spectra of bio-oil samples suffer from severe signal overlap. Derivatisation, where fluorine-containing compounds are reacted with the carbonyl groups, is preferred. Sparser ^{19}F NMR spectra provide both estimates of the total carbonyl content and quantification of the different carbonyl functional groups present. Benchtop NMR equipment is cheaper, smaller, uses weaker magnets, requires no cryogens and less maintenance, and does not require deuterated solvents [1].

However, the derivatisation reactions often rely on harmful and increasingly restricted solvents, such as DMF. By using ethyl lactate instead, the reaction is rendered safer and more sustainable, while still obtaining good quality NMR results. It is also possible to increase the amount of water in the solvent mixture, further reducing the environmental impact, user risks, and cost of the analysis [2].



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APC - D2 - O16
Novel electroanalytical methods for monitoring of environmental carcinogens

Jiri Barek[1]
[1]Charles University, Faculty of Science, Dept. of Analytical chemistry, UNESCO Laboratory of Environmental Electrochemistry, Czech Republic
Email : Barek@natur.cuni.cz

There is an ever-increasing demand for monitoring of environmental carcinogens and modern electroanalytical methods play a significant role in this field because of their portability, sensitivity, selectivity, low cost, and compatibility with green and white analytical chemistry and large-scale high throughput on site monitoring[1]. Possibilities and limitations of flow-through analytical systems with electrochemical detection are discussed in the IUPAC technical report[2] on project of Division V of IUPAC[3]. Most engineered nanoparticles can have genotoxic properties as well and their monitoring in the environment is disused in IUPAC technical reports[4,5]. This presentation is focussed on novel electrode materials (e.g. O-terminated pristine micro-/ultrananocrystalline boron-doped diamond[6], laser reduced graphene oxide decorated with silver nanoparticles[7], biochar based carbon[8] or silver amalgam[9] both in batch, flow or batch injection arrangement. Attention will be paid to education of modern electroanalytical methods[10] as well.

Acknowledgements: This work was financially supported by the Grant Agency of the Czech Republic (project GAČR 25-16569S). Material, technical and intellectual support of Metrohm.CZ (www.metrohm.com/cs-cz/) is highly appreciated.

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APC - D2 - O17

Nontarget screening and PhotoTOP assay to characterize PFAS in AFFF contaminated sites

Christian Zwiener[1], Catharina Capitain[1], Melanie Schüßler[1]
[1]*Eberhard Karls University Tübingen, Environmental Analytical Chemistry, Germany*

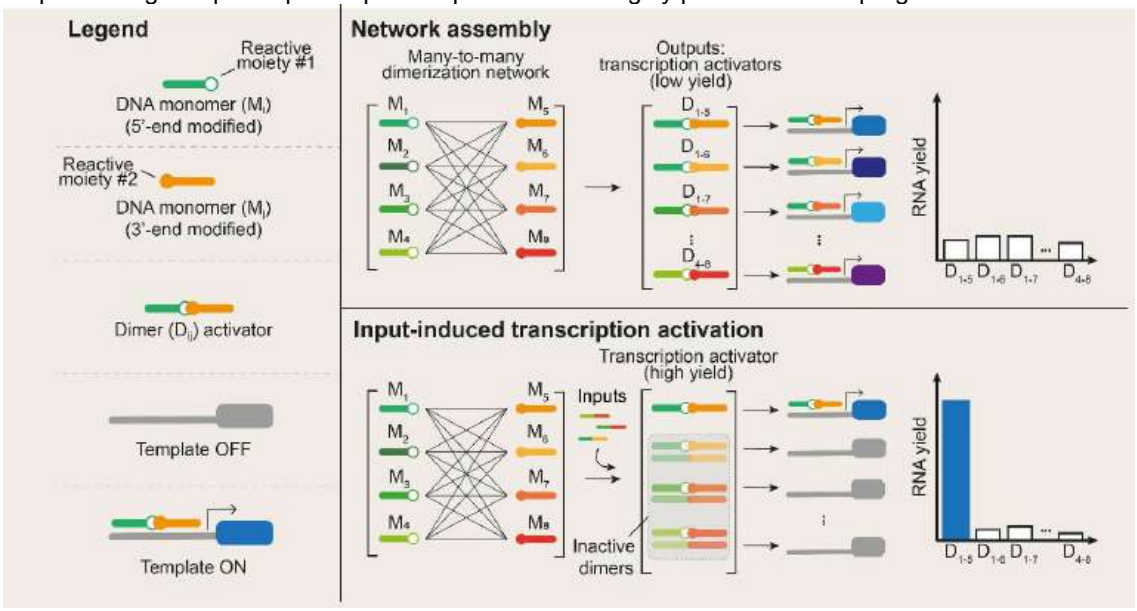
The analysis of PFAS in environmental samples is very challenging because of their diverse physical/chemical properties and the high number of individual PFAS compounds. Therefore, nontarget screening (NTS) approaches are highly attractive and provide promising results. For assessment of risks and long-term behaviour of PFAS in contaminated sites, semi-quantification and identification of transformation products and their formation kinetics is furthermore required.
In this work we present data from an AFFF contaminated soil site from a large fire event in 2008 in southwest Germany. Based on NTS and data prioritization and evaluation using our software tool PFAScreen we identified a much larger extent of PFAS contaminants than previously known: 124 PFAS and their transformation products from 42 subclasses at confidence levels for identification between 1 and 3. These included anionic, cationic, and zwitterionic substances with 3 to 14 perfluorinated carbon atoms. Only 28 PFAS could be quantified based on standard calibration functions. We therefore developed and applied a semi-quantification method based on matrix-matched average calibration curves of suitable authentic standards taking four different functional and/or ionization groups into consideration: carboxylic acids, sulfonic acids, sulfonamides, and cationic PFAS. We achieved a median prediction error of 2.2x, at a range between 1.3x and 5x. This showed that in the topsoil of the contamination cationic and zwitterionic PFAS dominate, that semi-quantified PFAS more than doubled the sum concentration of quantified PFAS in soil (7.3 µg/g) and that the total sum finally explains completely the extractable organic fluorine (EOF) of the contamination. To predict the long-term behaviour of the contamination we performed photocatalytic oxidation processes (PhotoTOP) and identified potential intermediates and final oxidation products by target and NTS and investigated their transformation kinetics. The results provide insight into the occurrence, behaviour and persistence of PFAS in contaminated soil and their potential fate in the environment.

We acknowledge BMFTR (Federal Ministry for Research, Technology and Space) for funding of the project PFClean (02WGW1665C).

APC - D2 - O18
Covalent DNA-based dimerization networks to control *in-vitro* transcription

Miriam Quattrociocchi[1], Simone Brannetti[1], Erica Del Grosso[1], Francesco Ricci[1]
[1]*Dept. of Chemical Sciences and Technologies, University of Rome "Tor Vergata", Italy*

Living systems offer multiple examples of how fundamental functions can emerge from the interaction of molecular networks [1]. One such example is given by the competitive protein dimerization networks, in which monomers of proteins can interact to each other to form a wide library of possible output dimers. The upregulation of certain dimers can play a critical role in activating specific downstream biological pathways [2]. Here, we have recreated these naturally occurring networks by using synthetic DNA as an engineering material. To do this, we designed a competitive DNA dimerization network composed of DNA monomers functionalized with reactive groups that can covalently bond to each other and create a combinatorial library of DNA dimer outputs [3]. By introducing specific DNA inputs that selectively sequester monomers, we can drive the formation of a desired DNA dimer, which activates a specific *in-vitro* transcription system. This method is highly versatile, allowing a precise modulation of transcriptional output by tuning the size of the network and the composition of input strands. Moreover, the programmability of the DNA-based dimerization networks facilitates orthogonal transcription of multiple fluorogenic aptamers using different enzymes. Finally, we were also able to control complex pathways such as an enzymatic cascade. These DNA networks provide a platform for performing complex input-output computations in a highly predictable and programmable manner.



DNA-based dimerization network to control in-vitro transcription

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APC - D2 - O19
Combining flow-induced dispersion and native mass spectrometry for biomolecular analysis

Jonathan Eisert[1], Edvaldo Maciel[1], Frederik Lermyte[1,2]
[1]TU Darmstadt, Germany; [2]University of Antwerp, Belgium

The application of mass spectrometry to protein analysis has led to tremendous progress in biological science; however, there is still a pressing need for further methodological improvements. One of the most exciting developments in recent years has been the progress made with so-called native mass spectrometry, in which noncovalent protein complexes remain bound during ionisation and transfer into the gas phase. Through measurement of the mass of the intact complex(es), sometimes augmented with gas-phase fragmentation and mass measurement of the resulting products, important insights have been obtained in the stoichiometry and stability of protein-protein complexes, as well as (for example) binding of natural or artificial ligands, and the action of novel drug moieties such as molecular glues, which selectively modulate protein-protein interactions. Despite this tremendous potential, widespread adoption of native mass spectrometry is hindered by its incompatibility with non-volatile salts and traditional biological buffers, as these compounds lead to loss of sensitivity and extensive adduct formation. This fact typically necessitates a separate sample preparation workflow to other biochemical assays; furthermore, the use of non-traditional buffers raises questions about the interpretation of results, especially if proteins spend a long time in such buffers. Here, we present a versatile approach that exploits dispersion physics within a laminar flow through a capillary to separate species based on their hydrodynamic radii. In one implementation, we achieved ultrafast buffer exchange of proteins, protein-protein and protein-ligand complexes, and double-stranded DNA from traditional, high-salt buffers. Signals were detected in just 30 seconds and each experiment took approximately 2 minutes in total. In a different variant, exploiting Taylor dispersion, experiments took approximately 10 minutes, but allowed for simultaneous buffer exchange and hydrodynamic radius measurement of analytes. These methods use only aqueous solutions, are flexible and easily adopted, and can be tuned to the desired information and available equipment.

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APC - D2 - F01

Graph-based clustering of isotopic patterns in high-resolution MALDI-MSI using matrix distances

Teresa Scovacricchi[1,2], Alba Alvarez-Martin[3,1], Bertrand Thomas[2], Koen Janssens[1], Caroline Tokarski[2]
[1]AXIS Research group, NANOlab Center of Excellence, University of Antwerp, Belgium; [2]University of Bordeaux, CNRS, Bordeaux Proteome, France; [3]Conservation and Science, Rijksmuseum Amsterdam, The Netherlands

High-resolution MALDI mass spectrometry imaging (HR-MALDI-MSI) generates highly complex datasets, in which thousands of mass channels are recorded for each spatial pixel. While this capability enables the detection of subtle chemical features, it also poses major challenges for data interpretation, particularly in samples containing elements with pronounced isotopic patterns. In such cases, isotopic redundancy inflates data dimensionality and complicates feature selection in conventional peak-based or intensity-driven workflows.

Numerous software solutions have been developed for HR-MALDI-MSI data treatment, often relying on peak picking, chemometric methods, and visualization tools such as Kendrick mass defect (KMD) plots to identify chemically related ion series. Building on these established concepts, this contribution proposes a clustering strategy that explicitly exploits isotopic relationships through matrix-distance analysis.

The method relies on the selection of specific m/z distance ranges corresponding to isotopic peak spacing within each pattern. Based on these distances, a graph is constructed in which nodes represent mass features and edges encode isotopically meaningful proximity. Graph-based clustering then yields groups corresponding to isotopic clusters. From each cluster, a representative signal—defined as either the lowest m/z or the most intense peak—is selected to generate a reduced, chemically meaningful dataset.

The resulting simplified mass lists are subsequently visualized using Kendrick mass defect plots[1], enabling clearer pattern recognition and more straightforward chemical formula assignment. Application to HR-MALDI-MSI datasets containing significant isotopic contributions demonstrates improved robustness, reduced spectral redundancy, and enhanced interpretability of spatial ion distributions.

By integrating graph theory, chemically informed distance metrics, and Kendrick-based visualization, this strategy bridges classical chemometrics and modern data-driven analysis, offering a transparent alternative to black-box approaches and supporting the generation of trusted, interpretable data from high-dimensional analytical measurements.

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APC - D2 - F02

High-sensitivity UHPLC-MS/MS multi-residue analysis of pharmaceuticals in aquatic systems: Methodological advances for environmental risk and AMR assessment

Guglielmo Pacchione[1,2], Alessandro Bollella[1,3], Federica Nigro di Gregorio[1]

[1]National Centre for Water Safety (CeNSiA), Italian National Institute of Health, Italy; [2]University of Rome "Sapienza", Dept. of Chemical Science, Italy; [3]University of Rome "Sapienza", Dept. of Environmental Biology, Italy

Pharmaceuticals are increasingly recognized as a major class of emerging contaminants in aquatic environments, particularly in surface waters and wastewater-impacted systems. Despite their generally moderate environmental persistence and occurrence at trace levels, their continuous release leads to chronic exposure, raising concerns about long-term ecological effects. In recent years, the inclusion of several antibiotics in the European Union Watch List has highlighted the relevance of pharmaceutical pollution, particularly in relation to the environmental presence and spread of antimicrobial resistance (AMR), identified by the WHO as a critical global health threat. Beyond antibiotics, other therapeutic classes such as NSAIDs, antidepressants… can interfere with key physiological processes in aquatic plants, microalgae and fish, inducing community-level alterations and sub-lethal effects.

The aim of this work was to develop and validate a robust, high-sensitivity UHPLC-MS/MS multi-residue analytical strategy capable of simultaneously determining pharmaceuticals and metabolites at trace levels in complex aquatic matrices, while ensuring applicability to environmental monitoring and risk assessment frameworks. Method development was specifically designed to address analytical challenges posed by environmental samples, including matrix complexity and the wide physicochemical diversity of target compounds. A UHPLC-MS/MS method was developed and validated for the simultaneous determination of 26 pharmaceuticals and metabolites belonging to critical therapeutic classes, including beta-lactams, macrolides, fluoroquinolones, sulphonamides, lincosamides and diaminopyrimidines, as well as NSAIDs, antifungals, and anti-depressants.The analytical workflow involved rigorous optimisation of chromatographic conditions, electrospray ionisation in positive mode(ESI+/) and Multiple Reaction Monitoring parameters. To ensure maximum sensitivity and selectivity, different sample pre-treatment approaches were comparatively evaluated, including filtration with metal cation chelation followed by direct injection, online SPE and offline SPE. The validated method demonstrated high analytical performance, with limits of detection (LOD) and quantification (LOQ) in the ng/L range, strong linearity ($R^2 > 0.98$) and recoveries exceeding 75% for most analytes.Supporting regulation and understanding AMR environmental risk.

APC – D2 – F04

Ion mobility high-resolution mass spectrometry (IM-HRMS) – An emerging technique facilitating the analysis of environmental contaminants and their metabolites

Lidia Belova[1], Maosen Zhao[1], Mikel Musatadi[1,2], Maarten Roggeman[1], Giulia Poma[1], Fatima den Ouden[1], Alexander L.N. van Nuijs[1], Adrian Covaci[1]

[1]Toxicological Center, University of Antwerp, Antwerp, Belgium; [2]Dept. of Analytical Chemistry, University of the Basque Country (UPV/EHU), Leioa, Spain

Ion mobility high-resolution mass spectrometry (IM-HRMS) presents an advanced separation technique with applications vastly increasing in recent years. It allows the separation of ions based on shape and size, providing an additional separation dimension. From measured mobilities, collision cross section (CCS) values can be calculated providing an additional identification parameter in HRMS-based suspect screening. These advantages are of special interest for the identification of environmental contaminants in exposomics studies, often facing complex sample matrices and low annotation confidence due to limited coverage of emerging contaminants by existing reference spectral libraries.

This presentation describes two of our recent IM-HRMS applications in the analysis of emerging environmental contaminants. The first study focused on the utilization of CCS values for improved compound annotation in indoor dust samples collected in Flemish kindergartens. Despite increasing use of alternative plasticizers, phthalates remained among major annotated contaminant classes showing the highest detection frequencies and semi-quantified concentrations. Detected phthalates displayed extensive homologue series with side chains ranging between C_1 and C_{12}. Annotations confidence of homologue series was vastly improved based on CCS-*m*/*z* trendlines describing the relationship between CCS value and mass-to-charge (*m*/*z*) ratio. Homologue series showed characteristic trendlines with CCS values of suspect phthalate homologues falling within the 90th percent confidence interval calculated for the CCS-*m*/*z* trendline (Figure 1).

The second study focused on the use of a human liver microsome based *in vitro* model for the identification of metabolites of quaternary ammonium compounds – another major class of contaminants observed in the indoor environment. Characteristic changes in CCS values following metabolism reactions were observed and confirmed *in vivo* after the analysis of human urine samples. This confirmation improved the annotation confidence of metabolites and is expected to facilitate metabolite annotations for other contaminant classes.

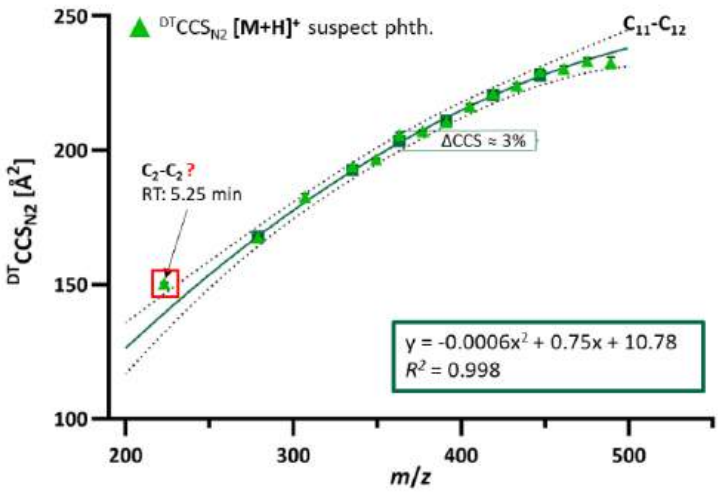

Fig. 1. CCS-*m*/*z* trendline describing the relationship between collision cross section (CCS) value and mass-to-charge (*m*/*z*) ratio. Dark-green squares represent CCS values calculated from phthalate reference standards. The corresponding CCS-*m*/*z* trendline was fitted using a 2nd order polynomial function for which the equation and correlation coefficient are displayed in the dark-green box. The 90th percent confidence interval is shown with dotted lines. CCS values obtained for suspect phthalates are displayed in light green. Datapoints falling outside the confidence interval were identified as false positive annotations (marked in red).

APC - D3 - O02

Application of a new monomer sensor for the fluorimetric detection of cadmium ions: Preparation of modified electrodes with fluorescent ion-imprinted polymers

Ouassim Boukaroum[1], Mélina Chebaiki[2], Erwann Ginoux[3], Jean-Luc Boudenne[1], Bruno Coulomb[1], Fabien Robert-Peillard[1], David Evrard[3], Olivier Reynes[3], Pierre Gros[3], Véronique Lenoble[4], Farah Ibrahim[2], Catherine Branger[2]

[1]Aix Marseille Univ, LCE, France; [2]Univ Toulon, MAPIEM, France; [3]Univ Toulouse, Lab Genie Chim, CNRS, INPT,UPS, France; [4]Aix Marseille Univ, Univ Toulon, CNRS, IRD,MIO F, France

Contamination of aquatic environments by heavy metals is a major concern in the scientific community and for societal issues. Monitoring of cadmium ions in water samples has attracted particular attention due to toxicity issues. Many molecular fluorescent sensors have been proposed to detect cadmium ions in water samples[1], with selectivity issues which often arise in real environmental samples, where concentrations of potentially interfering elements can be much higher than those of the target metal. Ion-imprinted polymers (IIPs) are material that can improve selectivity to a given target ion[2], and fluorescent IIPs can be synthesized with a monomer derived from a fluorescent chemosensor[3].

In this study, a modified quinoline-based molecule with a terpyridine group as recognition unit was implemented for the fluorescent detection of cadmium ions[4]. This type of fluorescent probe was first studied in liquid phase (dissolution of the probe in an organic solvent and addition to an aqueous solution of cadmium ions), by comparing the non-modified quinoline-based molecule with its monomer derivatives. Synthesis of these chemosensors and their fluorescence detection properties will be first described, with a special focus on the comparative sensitivity and selectivity (for cadmium ions compared to other cations) of these probes.

The monomer derivatives were then applied for the preparation of modified electrodes functionalized with fluorescent IIPs. Influence of various parameters were studied for the preparation of the modified electrodes: functionalization of the electrode surface, monomer/crosslinker ratio, nature of the crosslinker, choice of polymerization solvent… The fluorescence detection properties of IIPs will then be described and compared to the monomer sensor, with a special emphasis on cadmium/zinc selectivity. This study paves the way for the implementation of a dual detection method for cadmium with electrochemical and fluorescence sensing on electrodes[5].

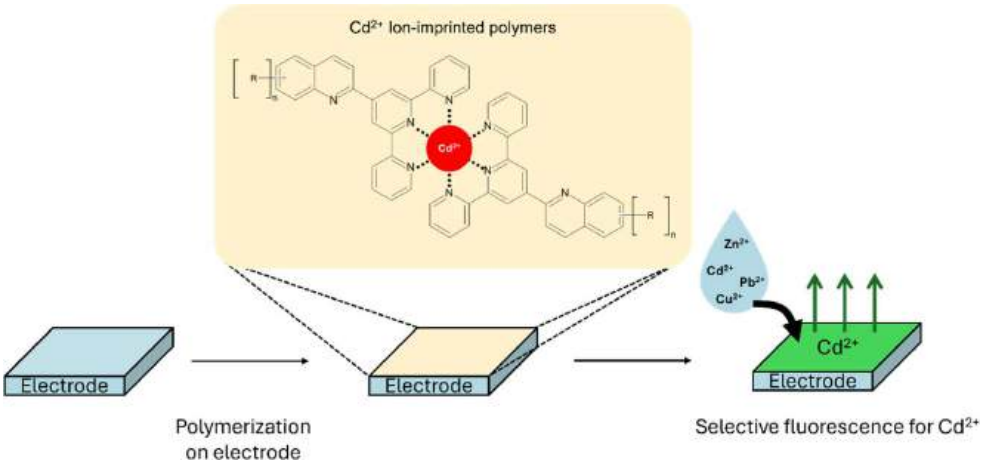

Fig. 1. Schematic illustration of Cd^{2+} selective fluorescent detection using functionalized electrodes incorporating fluorescent ion-imprinted polymers (IIPs) based on a quinoline-derived molecule modified with a terpyridine group.

Acknowledgements: this study has received funding from the French Research Agency (project « IDEALWATER », ANR-22-CE04-0003).

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APC - D3 – O03

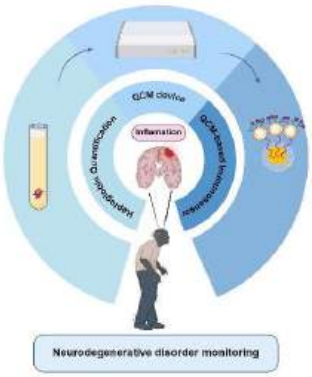
A label-free QCM immunosensor based on hyaluronic acid–coated solid lipid nanoparticles for non-invasive haptoglobin monitoring in neuroinflammation

M. Lettieri[1], L. Talarico[1], M. Consumi[1], I. Clemente[1], G. Gabricci[1], A. Magnani[1], E. Landi[2], A. Fort[2], V. Vignoli[2]
[1]Dept. of Biotechnologies, Chemistry and Pharmacy, University of Siena, Italy; [2]Dept. of Information Engineering and Mathematics, Italy

Neurodegenerative diseases (NDs), exhibit distinct molecular mechanisms but share common pathological hallmarks such as dopaminergic neuron degeneration and neuroinflammation. These processes are closely linked to chronic inflammation and oxidative stress, which correlate with elevated levels of systemic biomarkers like haptoglobin (Hp), an acute-phase inflammatory glycoprotein, and, consequently, with ND progression[1,]. However, current Hp detection methods (ELISA, nephelometry) are costly, invasive, and time-consuming, while conventional ND biomarkers (e.g., tau, amyloid-β) require invasive cerebrospinal fluid (CSF) sampling. To address this, we developed the first quartz crystal microbalance (QCM)-based immunobiosensor for rapid, non-invasive Hp quantification in human serum.

The immunosensor integrates an in-house QCM-R device for dual high-resolution frequency/resistance measurements. Fabrication involved functionalizing the quartz surface with a thiolated polyethylene glycol amine (SH-PEG-NH_2) self-assembled monolayer, followed by immobilization of hyaluronic acid coated solid lipid nanoparticles (HA-SLNs). HA-SLNs, here used for the first time in biosensor application, were designed to enhance surface stability, antibody loading capacity, and sensitivity. Subsequent steps included covalent attachment of Hp antibodies and ethanolamine blocking to minimize nonspecific binding. The biosensor demonstrated robust analytical performance, achieving high sensitivity (612.10 ± 28.14 μg mL^{-1}), reproducibility (CV_{av} % = 0.50 %), selectivity, and exceptional limits of detection (0.06 ± 2.90 x 10^{-3} μg mL^{-1}) and quantification (0.21 ± 9.70 x 10^{-3} μg mL^{-1}). Layer-by-layer surface modifications were validated using atomic force microscopy (AFM), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and electrochemical impedance spectroscopy (EIS).

This study pioneers the use of piezoelectric immunosensors for Hp detection, bridging a critical gap in ND diagnostics. By eliminating the need for invasive CSF sampling and complex instrumentation, this platform could offer a cost-effective, user-friendly solution for early ND diagnosis and therapeutic monitoring.



Acknowledgments: This study was cofunded by the European Union - Next Generation EU, in the context of The National Recovery and Resilience Plan - Investment 1.5 Ecosystems of Innovation, Project Tuscany Health Ecosystem (THE), Spoke 3 993 “Advanced Technologies, Methods and Materials for Human Health and Well -Being ” , ECS00000017, CUP: 995 B63C22000680007.

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APC - D3 - O04
Enzyme nanocapsules as robust biosensors

Dhanjai[1]
[1]*Dept. of Chemistry, University of Allahabad, India*
Email: dhanjai83@gmail.com

Biomolecules such as glucose, adrenaline, dopamine are integral elements of living organisms and control many biochemical functions of the body. Such biomolecules are generally termed as biomarkers for body metabolite or disease detection. Increasing imbalance in the natural metabolism of human body results in irregular secretion/absorption and alteration in biomolecule concentration which may lead to various genetic, metabolic, and cancerous diseases. Therefore, there is a great need for highly sensitive, accurate and stable detection platforms for their fast and specific detection. My research focusses on the development of advanced biosensing devices based on new generation nanostructures and biomaterial for fast screening of disease biomarkers towards point-of-care diagnostics and for other applications such as food safety and environmental protection.
The present study demonstrates the use of highly stable single-molecule enzyme nanocapsules (SMENs) instead of traditional native enzyme as biorecognition element in enzyme-based biosensors. The main purpose of this study is to resolve the major obstacle and challenge in the biosensor field, i.e., the poor stability of enzyme-based biosensors, including thermal stability, organic solvent tolerance, long-term operational stability, etc. For this purpose, highly active and robust SMENs of glucose oxidase (GOx, as a model enzyme) were synthesized (nGOx) using an in-situ polymerization strategy in an aqueous environment and used for the detection of glucose. The detection strategy can be easily generalized for sensing of other disease and metabolic biomarkers.

APC - D3 - O05
Exploring PFAS as a new source of chemical exposure in cosmetic formulations

Bernat Oró-Nolla[1], Christian Zwiener[1]
[1]*Environmental Analytical Chemistry, University of Tübingen, Germany*

Per- and polyfluoroalkyl substances (PFAS) are widely used in cosmetics to improve durability, brightness, skin penetration, and oleophobic properties, particularly in hair-care formulations [1], since PFAS are effective emulsifiers and lubricants. Since 2013 [2], mostly precursors as polyfluoroalkyl phosphate esters (PAPs) have been detected at µg/g levels across Japan, Denmark, Sweden, France, and North America [3]. Toxicological data remain scarce, and regulatory oversight is limited because in Europe, additives < 1% are not listed, but 76% of certain PFAS are dermally bio accessible [4]. Our hypothesis is that cosmetics containing polyethylene glycols (PEGs), widely used as co-formulants, may incorporate bis(trifluoromethylsulfonyl)imide (NTf_2), recently detected in wastewater [5] and human hair [6]. We analysed 30 samples containing PEGs. One product free of fluorinated chemicals was employed as a fortified quality control at 100 ng/g to assure reproducibility and robust concentrations (n=3). 100 mg were extracted using NaOH and MeOH. The extract was neutralized and cleaned-up with activated carbon and acetic acid and finally preconcentrated. Liquid chromatography (Agilent C_{18} Poroshell, 2.1 mm × 100 mm, 2.7 µm) was used coupled to a triple quadrupole MS for targeted analysis with 45 PFAS acquired in multiple reaction monitoring mode. NTf_2 was recovered at 93% (RSD=5%), proving a robust and reproducible methodology. In the cosmetics, NTf_2 was found in the ng/g range. Further unknown fluorinated chemicals in cosmetics will be identified, addressing a significant gap in exposure assessment and supporting future risk assessment and regulation.

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APC - D3 - O06

NMR and IR spectroscopies as alternative analytical methods for biopolymers without chromophore: Example of hyaluronic acid in dietary supplements and cosmetics

Yulia Monakhova[1,2], Fabienne M. Lang[1], Klaudia Adels[1], Julia Wang[1]
[1]University of Applied Sciences Aachen, Germany; [2]Saratov State University, Russia

In recent years hyaluronic acid (HA) has attracted considerable attention due to its natural origin, biodegradability, immunosuppressive, and moisturizing properties. Today, HA is used in dietary supplements, eye drops, shampoos, facial creams, and other so-called “anti-aging” products. The main analytical obstacles include the broad variation in molecular weight and the poor UV absorption of HA, as well as the need for derivatization or enzymatic treatment and the requirement for complex and expensive analytical instrumentation (e.g., LC/MS).

Low-field NMR and ATR-IR methods were first employed for the analysis of dietary supplements. ATR-IR-based analysis were performed without sample preparation by multivariate regression. In low-field 80 MHz NMR, hyaluronic acid was detected after acidic hydrolysis (80 °C, 0.1 M HCl, 2 hours) (Fig.1). Quantitative analysis was carried out using nicotinamide (NSA) as an internal standard. For direct quantification, high-field (HF) NMR experiments were required.

The developed HF NMR method was also tested on “anti-aging” products. For sample preparation, HA was extracted with methanol from the eye drops or with CHCl3/MeOH mixture (1:2) from the remaining matrices (cremes, serums, and shampoos). In both cases precipitates were isolated by centrifugation and evaporation of the remaining solvent. The dried pellets were then dissolved in D_2O. The intraday precision values were below 0.4% and 4% without and with sample preparation, respectively. The limits of detection and quantification of this method were 0.02 mg/mL and 0.07 mg/mL HA, respectively. Recovery rates between 99-108% and 85-89% for eye drops and creams, respectively, were achieved.

In conclusion, NMR and IR spectroscopy serve as a simple and efficient quality control tool for HA in complex samples.

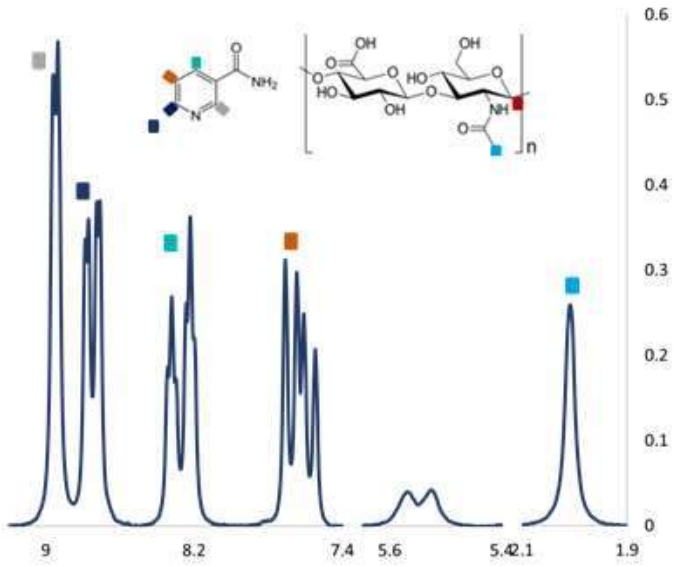

Fig.1. LF NMR spectrum of hydrolysed HA sample.

This study was supported by the German Federal Ministry of Research, Technology and Space (BMBF), Grant 13FH522KA2.

APC - D3 - O07

Batch injection analysis with electrochemical detection as a useful tool in food and pharmaceutical practice

Ľubomír Švorc[1], Marek Haššo[1], Emma Pochová[1], Monika Čerňanská[1]
[1]Institute of Analytical Chemistry, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Slovakia

Batch Injection Analysis (BIA) combined with electrochemical detection represents a promising analytical technique characterized by high analysis throughput, low consumption of samples and reagents, and straightforward implementation[1]. It enables direct and reproducible measurements without the need for laborious sample pretreatment, making it particularly attractive for applications in food analysis and the pharmaceutical industry.

This contribution will focus on optimization strategies applied during the development and validation of novel analytical methods using a BIA system coupled with electrochemical detection. Special attention will be paid to selected practical applications, including the determination of pharmaceutical active ingredients and food additives[2,3] (Fig. 1). Overall, BIA with electrochemical detection emerges as an efficient, robust, and versatile tool for modern analytical practice, offering significant potential for routine analysis in food and pharmaceutical fields.

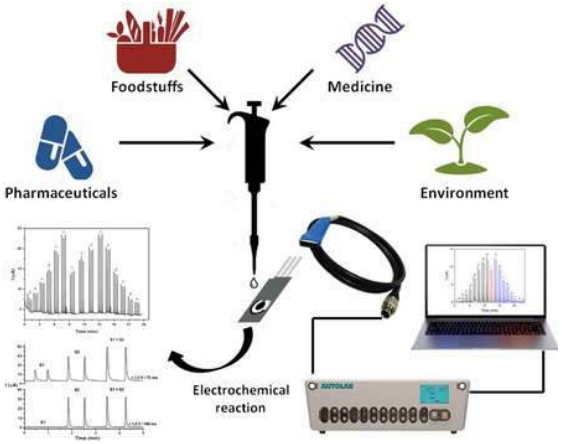

Fig. 1. Schematic illustration of BIA with electrochemical detection and its applications in food, pharmaceutical, medical, and environmental analysis.

This work has been supported by the Scientific Grant Agency of the Ministry of Education, Research, Development and Youth of the Slovak Republic and the Slovak Academy of Sciences (VEGA No. 1/0036/24) and the Slovak Research and Development Agency under the Contract no. APVV-23-0066.

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APC - D3 - O08
Emulsifying properties of cetearyl olivate and sorbitan olivate in semi-solid cosmetic matrices

Marta Marzec[1], Iga Ledzińska[1], Izabela Nowak[1]
[1]Adam Mickiewicz University, Poznań, Faculty of Chemistry, Dept. of Applied Chemistry, Poland

Cetearyl olivate and sorbitan olivate are non-ionic emulsifying agents derived from olive oil fatty acids, widely used in cosmetic formulations due to their favorable physicochemical properties and natural origin. The present study focuses on the development and characterization of semi-solid cosmetic systems in the form of oil-in-water (O/W) emulsions intended for hand care applications, formulated using a natural emulsifier system Olivem® 1000 (based on cetearyl olivate and sorbitan olivate). Selected vegetable oils, namely jojoba oil, raspberry seed oil, and sweet almond oil, were incorporated as the lipid phase to enhance emollient properties and skin compatibility.[1] The formulations were characterised in terms of physicochemistry (pH, viscosity). A long-term stability study was also carried out using the multiple light scattering method (MLS, Turbiscan®) to identify instabilities invisible to the human eye, related to both particle migration (creaming, sedimentation) and particle size changes (flocculation, coalescence). Stability assessments were carried out to ensure that the products tested behaved correctly over their declared shelf life, under specified storage conditions, and during their normal use in the final packaging.[2] After an assumed three months, a normal pH value was recorded for the formulations obtained, as well as slight changes in their viscosity over time and under the influence of the specified storage temperature. The stability of the tested cosmetic formulations was determined independently of storage time and temperature, and the type of vegetable oil used ($\Delta BS<3\%$), except for samples stored at 45 °C, for which more pronounced changes were observed. Based on the results obtained, the developed hand care products were determined to be stable for the introduction of additional active substances and qualified for the following in the next stage of application tests.

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APC - D3 - O09

Extending SPE lifetime for accurate electrochemical detection of emerging environmental pollutants using machine learning-based data interpretation

Antonio Licheri[1], Francesco Siconolfi[2,3], Khitem Lahbacha[2,3], Luca Tari[2,3], Gabriele Cavaliere[2,3,4], Ciro D'Elia[2], Antonio Maffucci[2,3], Laura Micheli[1]

[1]Dept. of Chemical Sciences and Technologies, University of Rome Tor Vergata, Italy; [2]Dept. of Electrical and Information Engineering, University of Cassino and Southern Lazio, Italy; [3]Inst. of Nanomaterials and Nanotechnologies, European Uni. of Technology, EU; [4]University of Salerno, Italy

Screen-printed electrodes (SPEs) are widely used for in situ electrochemical detection because they are low-cost and portable. However, their analytical performance depends strongly on electrode stability. Fouling, surface degradation, and batch-to-batch variability reduce both precision and reproducibility, so SPEs are usually used only once, raising sustainability concerns, especially for large-scale monitoring[1].

Benzoquinone (BQ) and hydroquinone (HQ) were selected as model analytes, as both are redox-active emerging contaminants detected in natural and wastewaters and associated with oxidative stress effects in aquatic environments[2].

This work aims to extend SPE lifetime without compromising analytical precision for HQ and BQ detection in water samples by using machine-learning (ML) analysis for data interpretation. Chronoamperometry was chosen as quantification techniques and six different, HQ and BQ concentrations (5, 4, 3, 2, 1, and 0.5 mM) were analysed, performing 20 consecutive measurements on the same electrode. As expected, current decreased progressively due to surface degradation, confirming that traditional interpretation approaches fail under these conditions.

To evaluate SPE reusability, concentration recognition was reframed as a supervised classification problem using full chronoamperometric curves. A Kernel Naïve Bayes classifier was tested under two strategies: Static training and adaptive on-electrode retraining. For the first approach, training on repeated measurements from two electrodes per concentration and testing on a held-out device yielded mean accuracies of 84%. Majority voting across replicate predictions resulted in 100% correct assignments.

In the second approach, periodic retraining every four measurements achieved accuracies of 87%, again reaching 100% correct classification after voting.

These results show that ML-assisted chronoamperometry enables reliable SPE reuse without compromising analytical performance, addressing both sustainability and signal-drift limitations of conventional quantification methods.

Acknowledgements: The research leading to these results has received funding from the Project "SENS-AI, Environmental Sensing with Artificial Intelligence" CUP H53D23000520006 (Italian"Bando Prin 2022 - D.D. 104 del 02-02-2022" by MUR (2023-2025), Project ""Dress the future; novel combined wearable integrated system (Stargate)" CUP E53D22014620001 by MUR (2023-2025)(MUR-PRIN 2022 PNRR Decreto Direttoriale n. 1409 del 14-9-2022) and Grant MUR Dipartimento di Eccellenza 2023-27 X-CHEM project "eXpanding CHEMistry: implementing excellence in research and teaching".

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APC - D3 - O10

Chemometric optimization of a green DES-RP-DLLME method for total phenolic determination in cosmetic matrices

Yasemin Çağlar[1]
[1]*Giresun University, Turkey*

In this study, a green and efficient reversed-phase dispersive liquid–liquid microextraction (RP-DLLME) method based on deep eutectic solvents (DESs) was developed for the determination of total phenolic content in complex hydrophobic matrices. Phenolic compounds are important bioactive constituents widely present in food and cosmetic products; however, their determination is often challenging due to strong matrix interferences and the need for laborious sample preparation steps [1].

To overcome these limitations, a DES-based RP-DLLME approach was proposed as an environmentally friendly alternative to conventional extraction techniques [2]. The extraction process was optimized using a chemometric strategy, where Plackett–Burman design was first applied to screen the main experimental variables affecting extraction efficiency, followed by Central Composite Design (CCD) for response surface optimization. Key parameters, including extraction solvent volume, DES disperser volume, pH, and centrifugation conditions, were systematically evaluated.

Under optimized conditions, total phenolic compounds were efficiently transferred from the hydrophobic sample matrix into the aqueous phase and quantified by UV–Vis spectrophotometry. The proposed method demonstrated good sensitivity, satisfactory repeatability, and low solvent consumption, while significantly reducing chemical waste in accordance with green chemistry principles.

This study provides an original contribution to the literature, in which the use of a deep eutectic solvent (DES)–based RP-DLLME approach for phenolic analysis has been rarely reported, and demonstrates the high potential of this approach for the rapid and sustainable determination of bioactive compounds in complex matrices.

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APC - D3 - O11

Toward an innovative portable MicroNIR/chemometric strategy for the determination of disinfection byproducts in water

Tatsiana Pobat[1], Elena Papa[2], Gaia Rizzo[2], Giordano Putzolu[2], Federica Valeriani[1], Roberta Risoluti[2], Vincenzo Romano Spica[1]

[1]Dept. of Exercise, Human, and Health Sciences, University of Rome "Foro Italico", Italy; [2]Dept. of Chemistry, University of Rome "Sapienza", Italy

Rapid, onsite detection of disinfection by-products (DBPs) in water is essential to protect public health. Trihalomethanes (THMs) are among the most regulated DBPs [1, 2], typically monitored as the sum of four compounds, including chloroform ($CHCl_3$) and bromoform ($CHBr_3$), due to their toxicological impact [3]. Conventional chromatographic methods [4] require complex sample preparation, are time-consuming and unsuitable for real-time monitoring. Miniaturized near-infrared spectroscopy (MicroNIR) coupled with chemometrics offers a portable and "green" alternative [5].

In this study, MicroNIR/chemometrics platform was applied to aqueous solutions spiked individually with $CHCl_3$ and $CHBr_3$ at environmentally relevant concentrations (1-200 µg/L). Spectra were acquired using OnSite-W and PAT-L devices (in vial, static and flow modes). Principal Component Analysis effectively separated blanks from spiked samples, while Partial Least Squares Discriminant Analysis achieved near 100% specificity and non-error rate, with low root mean square errors. Partial Least Squares Regression provided accurate quantification with detection limits around 1 µg/L, particularly in PAT-L flow mode. Preliminary tests with co-present $CHCl_3$ and $CHBr_3$ suggest the platform's potential for simultaneous THMs assessment. Although additional validation tests are necessary before routine application, this novel MicroNIR/chemometric platform represents a promising portable, real-time, environmentally- and user-friendly strategy for DBPs monitoring in water, contributing to better public health protection.

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APC - D3 - O12

An AI-driven tool for the metabolic signatures of new psychoactive substance exposure within the NARCOSIS platform

Erika Castrignanò[1], Valentina Mongelli[2], Valentina Morciano[1], Ilaria Iacobellis[2], Michele Catacchio[2], Lucia Sarcina[1], Luisa Torsi[1], Eleonora Macchia[2]

[1]Dpto di Chimica, Università degli Studi di Bari Aldo Moro, Italy; [2]Dipto di Farmacia – Scienze del Farmaco, Università degli Studi di Bari Aldo Moro, Italy

The NARCOSIS project (Non-tArgeted foRensic multidisCiplinary platfOrm for inveStigatIon of drug-related fatalitieS) aims to establish a fast, robust, and harmonised diagnostic ecosystem for the investigation of drug-related deaths (DRDs), particularly due to NPS.[1] An AI-assisted toolkit for spectra management and data integration along with a shared, cross-organisational meta-spectra database will facilitate rapid and standardised detection of drugs of abuse. In the longer term, this framework will strengthen institutional responsiveness and inform evidence-based policymaking in relation to emerging NPS threats. The platform integrates analytical instruments technologies—including hyperspectral imaging, high-resolution mass spectrometry (HRMS) and novel sensing approaches—for both on-site and laboratory use, providing a comprehensive analytical foundation for forensic investigations.

Within this project, our study develops the metabolic tool capturing direct biomarkers associated with NPS exposure. The forensic detection of NPS remains particularly challenging due to their extensive structural diversity, the limited metabolic knowledge available for newly emerging compounds and the restricted availability of analytical reference standards, all of which constrain conventional targeted analytical workflows and hinder timely identification.

By using retrospective LC-HRMS data from forensic laboratories and sensorgrams acquired by a a newly developed biosensor, the tool is trained by a machine-learning model to link metabolic signatures to NPS exposure. This integration presents analytical challenges, notably the harmonisation of LC-HRMS data derived from diverse instruments and methodological workflows across forensic laboratories. End users will further contribute to the validation phase of the AI-assisted tool by incorporating new datasets associated with emerging NPS. Overall, this strategy supports the discovery of previously uncharacterised biomarkers and metabolic pathways, enhancing the capability of forensic systems to respond to the evolving NPS landscape.

Acknowledgements: This research is funded by the European Union's Horizon Europe research and innovation programme (Civil Security for Society) under grant agreement No 101168195.

[1]https://www.narcosis-project.eu/

APC - D3 - O13

Large-scale evaluation of semiempirical quantum mechanical EI-MS prediction for toxic compounds

W. Rojas[1], A. Křenek[2], H. Hecht[1], E. Price[1]

[1]RECETOX Centre, Faculty of Science, Masaryk University, Czech Republic; [2]Institute of Computer Science, Masaryk University, Czech Republic

The limited availability of high-resolution electron ionization (EI) mass spectral libraries for environmental chemicals restricts accurate compound annotation. Many environmental chemicals are not commercially available, and existing experimental libraries lack chemical diversity, further limiting identification capabilities. Computational approaches, such as machine learning models, provide an alternative but require large, high-quality training datasets, which are scarce for high-resolution EI spectra. In contrast, quantum chemistry-based methods offer a data-independent approach by simulating ionization and fragmentation processes. However, their predictive accuracy across diverse environmental chemicals has not been systematically assessed. Additionally, previous studies have primarily compared predicted spectra to low-resolution commercial libraries rather than high-resolution experimental spectra, **thereby limiting robust evaluation of predictive performance**.

This study presents the first systematic evaluation of QCxMS prediction accuracy for a large set of high-resolution EI spectra of environmental chemicals. **The analysis was enabled by** an open-source, semi-automated workflow developed in our group for EI-MS spectral prediction, utilizing **a** semiempirical tight-binding parameterization embedded in QCxMS. Simulated spectra were compared to experimentally acquired high-resolution EI spectra to assess the influence of molecular flexibility, **the number of** rotatable bonds, and atomic electronegativity on prediction accuracy.

Among the 367 compounds analyzed, prediction accuracy negatively correlated with molecular flexibility, the number of rotatable bonds, and electronegativity, **while accuracy was higher** for rigid, planar molecules. Only a few analytes were predicted with sufficient accuracy for spectral matching. Moreover, the most abundant *m/z* values in predicted spectra rarely matched experimental data, highlighting a significant disconnect between simulated and actual fragmentation trajectories.

These findings emphasize the need to improve QCxMS performance to advance spectral prediction for non-targeted environmental compound identification. Future work will focus on refining **the** semiempirical parameterization for **this** molecular set.

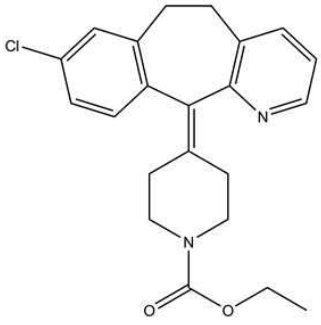
APC - D4 - O01

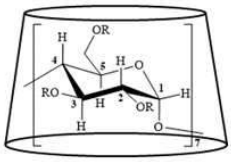
Influence of cyclodextrins on loratadine stability and structural characterization of degradation products by HR MS/MS

Marijana Pocrnić[1], Mario Jug[2], Nives Galić[1]

[1]Faculty of Science, University of Zagreb, Croatia; [2]Faculty of Pharmacy and Biochemistry, University of Zagreb, Croatia

Loratadine (LOR) is a second-generation antihistamine used to treat allergy symptoms such as allergic rhinitis and urticaria. According to the Biopharmaceutical Classification System, it is classified as a Class II drug due to its low solubility and high permeability.[1] Cyclodextrins (CDs) are able to form inclusion complexes with various molecules, affecting their solubility and stability. Traditional solution-based methods of inclusion complex preparation in the solid state often require the use of organic solvents that are difficult to remove and can remain as impurities in the prepared products, affecting their safety. Grinding has proven to be an effective, fast, sustainable, and eco-friendly method for inclusion complex preparation.[2] Considering the positive effect of β-CD and its derivatives, hydroxypropyl (HP-β-CD), randomly methylated (RM-β-CD) and sulfobuthylether sodium salt (SBE-β-CD) on the loratadine solubility demonstrated in our previous study[1], solid binary systems of LOR and CDs were prepared by grinding at 1:1 and 1:2 stoichiometric ratios. To study the effect of cyclodextrins on loratadine stability, forced degradation experiments were performed in acidic, basic and oxidative conditions. The rate of loratadine degradation was determined by a previously validated UHPLC-DAD method. The effect of cyclodextrins on loratadine stability in acidic and basic media was insignificant. However, although loratadine is relatively stable in the presence of hydrogen peroxide, in the presence of cyclodextrins higher level of degradation was observed, yielding several degradation products. Structures of observed degradation products were elucidated based on high-resolution mass spectrometry MS and MS/MS spectra, observing new, previously unreported degradation products.





β-CD	R = –H
HP-β-CD	R = –H or $–CH_2CH(OH)CH_3$; DS = 4.5
RM-β-CD	R = –H or $–CH_3$; DS = 12
SBE-β-CD	R = –H or $–(CH_2)_4SO_3Na$; DS = 6.5

Fig. 1. Structure of loratadine and cyclodextrins

This work was supported by the Croatian Science Foundation under the project number HRZZ-2022-10-6033

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APC - D4 - O02
Individual Marcus-type kinetics controls singlet and triplet oxygen evolution from superoxide

Soumyadip Mondal[1], Stefan A. Freunberger[1]
[1]*Institute of Science and Technology Austria, Austria*

Oxygen evolution from superoxide is critical in oxygen redox chemistry. Superoxide experiences a broad range of oxidizing conditions to liberate oxygen. Superoxide commonly undergoes disproportionation due to its instability in most environments, occurring in both protic[1] and aprotic environments with strong Lewis acids like Li^+ and Na^+ [2]. During disproportionation ($2\ O_2^- \rightarrow O_2 + O_2$) , one superoxide is reduced to peroxide while the other is oxidized to form dioxygen, which may be $^3O_2$ or $^1O_2$. Examples include cellular respiration[3] and batteries. Relative $^3O_2$ and $^1O_2$ yields and kinetics are therefore fundamental to these systems[4], yet what controls the spin state distribution remains unclear.
We found out that the driving force for superoxide oxidation to $^3O_2$ and $^1O_2$ oxygen determines spin state [5], following Marcus normal and inverted region behavior. $^1O_2$ becomes significant only when $^3O_2$ evolution kinetics slow in the inverted region. These results clarify inconclusive findings on $^1O_2$ formation from superoxide via chemical oxidants and proton or Lewis acid-driven disproportionation. Understanding $^3O_2$ and $^1O_2$ formation controls should enable strategies to suppress harmful $^1O_2$ in synthetic redox systems. The findings expand knowledge on electrogeneration of excited species and raise questions about differing maximum kinetics for ground and excited states, with implications for life sciences and energy storage.

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APC - D4 - O03

In situ SAXS investigation of microfluidic aggregation kinetics of lipid-based nanocarriers

Ilaria Clemente[1,2], Luigi Talarico[1,2], Giulia Gabbricci[1,2], Benedetta Marmiroli[3], Barbara Sartori[3], Aleksi Sutinen[4], Clement Blanchet[4], Agnese Magnani[1,2]

[1]Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena &CSGI, Italy; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy; [3]Graz University of Technology, Austria; [4]European Molecular Biology Laboratory (EMBL), Hamburg Outstation c/o DESY, Germany

The development of effective drug delivery systems for therapeutics and diagnostics is a challenging matter in nanomedicine. Lipid-based nanocarriers (LNPs) currently represent the emergent technology to achieve controlled drug release, target selectivity, and enhanced intracellular uptake[1]. Advances in the development of precision microfluidic devices allow high-throughput screening and optimization of synthetic parameters (i.e. chip geometry, flow velocity and ratios) and lipid/polymer compositions. Thus, highly reproducible nanovectors with desired structural and surface properties can be obtained. Nevertheless, a lack remains of systematic investigation of fundamental processes, i.e. mechanism and kinetic of assembly in conditions that closely mimic microfluidic assembly. These latter constitute crucial knowledge to control aggregation and stability, since the transient and metastable states influence the final equilibrium states. Moreover, knowledge of relevant synthetic parameters to obtain specific structural and dynamic properties is fundamental to optimize nanosystem development. In this work, microfluidic-synthetized LNPs were designed and optimized by employing varied molar fractions of lipid components and polymer coatings, and the structural evolution occurring during microfluidic mixing with a laminar flow was investigated with high spatiotemporal resolution. Static and Time-resolved synchrotron SAXS measurements using *in situ* microfluidic setup showed that the supramolecular assembly and dynamics depend not only on lipid composition, but on total flow velocity and aqueous/organic flow ratios as well (Figure 1). Supramolecular characterization was complemented by Dynamic Light Scattering and Zeta potential measurements. The fundamental understanding of the mechanism and kinetics of assembly of these systems is essential to control aggregation and stability, and correlate structural and dynamic properties to carrier functionality[2], thus obtaining suitable prototypes for clinics.

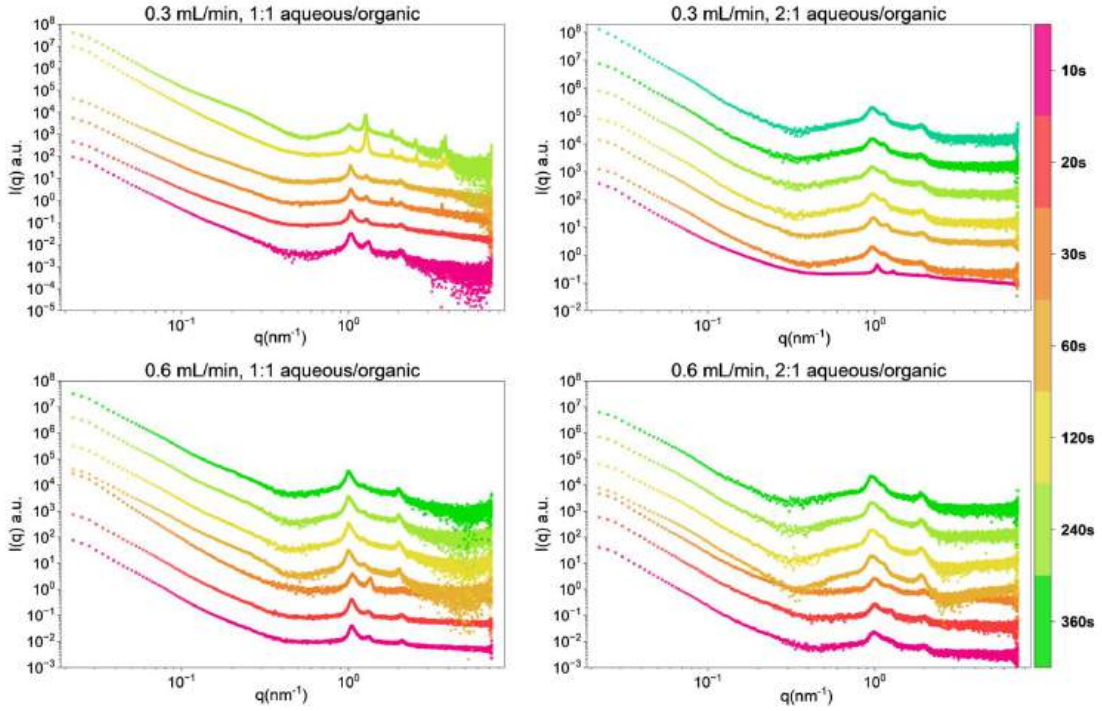

Fig. 1. Kinetics of LNPs assembly depending on total flows (mL/min) and aqueous/organic ratios.

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APC - D4 - O04

Probing light-triggered structural dynamics in lipid nanoparticles using Time-Resolved SAXS

Luigi Talarico[1,2,3], Ilaria Clemente[1,2,3], Giulia Gabbricci[1,2,3], Simone Cataldini[1], Elektra Mavromatidou[1], Jack Li-Yang Chen[1], Aleksi Sutinen[4], Clément Blanchet[4], Agnese Magnani[1,2,3]

[1]Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy; [2]Center for Colloids and Surface Science (CSGI), Italy; [3]National Interuniversity Consortium of Material Science and Technology, Italy; [4]European Molecular Biology Laboratory (EMBL), Hamburg Outstation c/o DESY, Germany

PEG-functionalized lipid nanocarriers are conventionally employed to obtain stealth delivery systems to avoid recognition from the immune system, thus reaching safely the target tissue. However, PEG surface coating also results in hindered fusogenicity with cell membranes and/or endocytic processes, as in the so-called PEG dilemma. A strategy to overcome this challenge is to synthetically design stimuli-responsive PEGylated amphiphiles, that can remove the PEG moieties by selective cleavage under monochromatic light. In this work, Time-Resolved Small Angle Xray Scattering (TR-SAXS) was used to investigate the kinetics and yield of PEG cleavage and possible nanocarrier structural transitions following the removal of the surface stabilizer. Alternatively, a photo switchable nanosystem, where a reversible cis-trans amphiphilic switch intercalated in the lipid membrane was used to provoke alterations and pore formation, leading eventually to drug release. This allowed us to investigate the extent of responsiveness of proposed systems, proving the effectiveness of the cleaving process and the nanocarrier stability to progressive coating loss. Information on the millisecond timescale of kinetics of responsiveness to light-triggered shedding of PEG coating was obtained, as well as temporary yield of surface modification and structural rearrangements to maintain stability upon polymer cleavage. Moreover, reversible alterations of the lipidic bilayer upon cis-trans isomerization of photoswithces was observed to be completely reversible upon irradiation with white light. The pre-formed lipid-based samples with the intercalated photoresponsive PEGylated amphiphiles were triggered with a near-UV monochromatic light source at 365 nm to irradiate samples during TR-SAXS acquisition. Complementary UV-VIS and fluorescence measurements of stimuli-responsive molecules were used to assess their process kinetics.

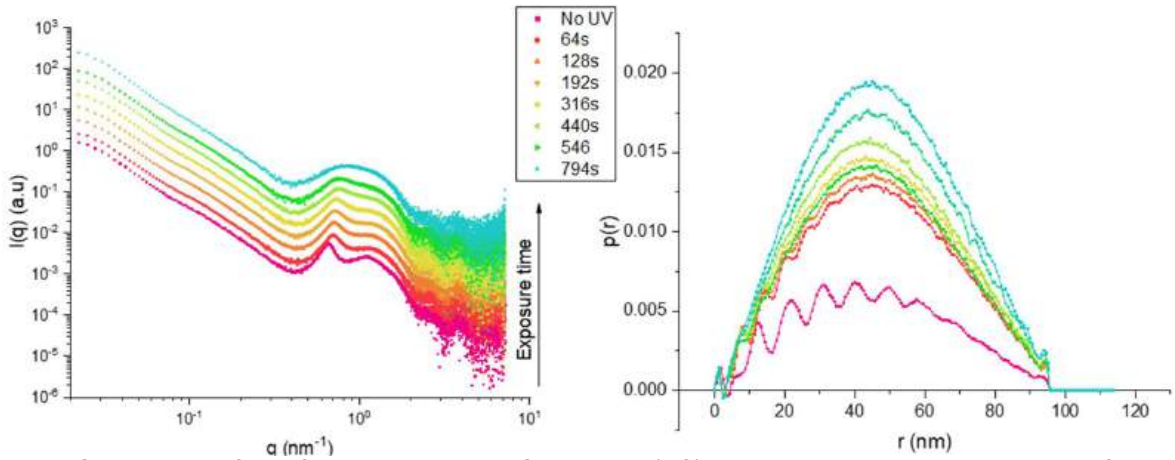

Fig. 1. Scattering profiles of photoactivated PEG cleavage (left) and corresponding pair distribution functions (right)

[1]J. A. Kulkarni, et al. *ACS Nano* **2018**, *12*, 4787−4795.
[2]X Yu et al. *ACS Nano* **2023**, *17*, 23, 23814–23828.

APC - D4 – O05

Interaction of copper with silanol nests in silicalite nanocrystals: Evidence from FTIR and CO adsorption study

Safaa Essid[1], Kateřina Knotková[1], Roman Bulánek[1]
[1]University of Pardubice, Faculty of Chemical Technology, Dept. of Physical Chemistry, Czech Republic

Pure silicalite serves as an effective host for copper nanoparticles (CuNPs) in various catalytic applications.[1] However, the high surface energy of CuNPs often leads to sintering and agglomeration, which reduces their active surface area and disrupts the unique electronic properties imparted by the zeolite microenvironment. Incorporating copper into the zeolite framework can mitigate these issues, as framework-bound copper species are less prone to sintering. In this study, silicalite was synthesized under tailored conditions in order to generate a particularly high concentration of internal silanol nests which serve as effective anchoring sites for copper species.

The structural features of the silicalite host were analyzed using FTIR spectroscopy, revealing two characteristic bands. A sharp band at 3740 cm^{-1}, assigned to isolated silanol groups on the external surface, and a broad band at 3510 cm^{-1}, attributed to hydrogen-bonded hydroxyl groups associated with internal defect sites such as silanol nests or Si–OH···OSi clusters.[2] Following the incorporation of 1–3 wt.% Cu via wet impregnation, a progressive decrease in the 3510 cm^{-1} band was observed. This decrease indicates a partial consumption of silanol nests, suggesting that copper species are being incorporated directly into these framework defect sites.

The nature of the anchored copper was further probed using CO-FTIR spectroscopy. A prominent band at 2131 cm^{-1}, corresponding to the ν (Cu^{+}–CO) stretching vibration, appeared in both reduced and non-reduced samples, confirming the presence of Cu^{+} stabilized within the silicalite framework. Furthermore, with increasing copper loading, CO adsorption isotherms were analyzed to estimate the size of copper species confined within or located in close proximity to the silicalite framework.

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APC - D4 - O06
Raman-MCR can be used to study solvation shells in particle dispersions

Taritra Mukherjee[1], Moreno Meneghetti[2], Martin Rabe[1]
[1]Max Planck Institute for Sustainable Materials, Germany; [2]University of Padua, Italy

Changes in the intermolecular interactions of interfacial water at particle-solvent interfaces can influence catalyst activity in many reactions, yet spectroscopic investigations remain limited due to experimental difficulties. Unlike spectral subtraction or bulk-phase replacement strategies, multivariate curve resolution (MCR) can enable the extraction of directly comparable bulk and solute-correlated spectra from the dispersions without disturbing the native environment. However, due to inherent limitations of MCR, a broad applicability of the technique on a class of systems cannot be confirmed without successful experiments on representative examples. Here, a methodology was established to implement Raman spectroscopy combined with MCR (Raman-MCR) as a reliable tool for probing solvation shells in aqueous particle dispersions.[1,2]
The methodology was first validated using aqueous dispersions of citrate-stabilised gold nanoparticles (Au NPs). The solute-correlated spectra revealed disruption of hydrogen-bonding networks in solvation shell. Control experiments using sodium citrate solutions and ligand-free pulsed laser ablated Au NPs confirmed that these changes arise from particle-water rather than citrate-water interactions. Control experiments with increasing temperature ruled out local laser heating artefacts, while comparative studies of gold and silver NPs demonstrated that an energy proximity between the nanoparticle plasmon resonance and the Raman laser emission wavelength does not change “how” the bulk and solute-correlated spectra differ, but does influence “how much” they differ. Electric field intensity enhancement simulations by finite element method supported this interpretation. The approach was further extended to non-metallic systems using, for example, zinc oxide and titanium dioxide particles, with phase-dependent interfacial behaviour observed for TiO_2.
This work establishes Raman-MCR as a robust, versatile tool to study solvation shell water in particle dispersions, also paving the way for reproducible comparative studies on catalyst materials.

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APC - D4 - O07

Flow-based automatic and miniaturized solid-phase extraction towards sample preparation and renewable sensors

Marcela A. Segundo[1], Diana R. Cunha[1], Sara R. Fernandes[1], Luisa Barreiros[1]
[1]LAQV/REQUIMTE, Faculty of Pharmacy, University of Porto, Portugal

Flow-based sample treatment, embedded in the principles of flow injection analysis, enables the precise management of solutions or suspensions within confined environments. By providing meticulous control over temporal and spatial parameters, these strategies significantly enhance reproducibility and facilitate the kinetic control of chemical processes.

This communication highlights recent developments in automated flow-based strategies designed to overcome traditional challenges in bioanalysis and pharmaceutical development, such as sorbent fouling, sample carryover, and analyte degradation. The implementation of Lab-on-Valve (LOV) devices combined with the bead injection (BI) concept is presented as a robust platform for automating solid-phase chemistry. Unlike conventional microfluidic devices, the BI-LOV approach allows for the microfluidic handling and renewal of beads, offering a high surface-to-volume ratio and real-time monitoring of solid-support phenomena. We discuss the online hyphenation of these systems with HPLC and MS detectors, addressing eluent compatibility and the assembly of immunoaffinity columns. Key applications demonstrate this versatility, including the reduction of ELISA protocol times from 2 hours to 5 minutes, and the rapid measurement of nanoparticle concentrations for quality control.[1-3]

Furthermore, the determination of drugs and endogenous compounds in complex matrices, such as plasma and urine, demonstrates the potential for handling real-world samples in a high-throughput, greener, and more efficient manner. Ultimately, these automated flow techniques represent a transformative approach to sample treatment, significantly improving accuracy and efficiency in the analysis of biopharmaceuticals and clinical samples.

Acknowledgments: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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[2]D.R. Cunha, S.S. Marques, P. Alves, G. Correia-da-Silva, M.B. Quinaz, M.A. Segundo, *Talanta* **2025**, 295, 128328.
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APC - D4 - O08
H_2 isotopologues chromatographic separation on metal oxides

Simone Puricelli[1], Antonio Sessa[1], Massimo Mella[1]
[1]*Università degli Studi dell'Insubria, Italy*

Hydrogen isotopes separation by conventional methods are hurdled by their nearly identical physiochemical properties. Quantum-based approachs exploiting mass-dependent effects in adsorption provide an effective mechanism for selective enrichment. Heterolytic chemisorption of hydrogen isotopologues has been observed on alkaline-earth oxides [1]. Thus, we theoretically investigate the reactivity of H_2 over Al_2O_3, Ga_2O_3, In_2O_3, and ZnO. Two adsorption sites were considered: (i) V1, corresponding to $M_{3c}O_{3c}$ for group-III oxides and $M_{4c}O_{4c}$ for ZnO; (ii) V2, corresponding to $M_{3c}O_{2c}$ for the group-III oxides and $M_{4c}O_{3c}$ for ZnO.
To assess the applicability of these oxides for isotope separation, we evaluated (i) adsorption selectivity $S(X_2/H_2)$, which depends on differences in ZPE contributions following adsorption, and (ii) the pressure at which adsorption sites are half-covered, p_{vap}, governed by the absolute adsorption energy. A larger ZPE gap leads to higher adsorption selectivity, whereas more exothermic chemisorption results in lower vapour pressure and higher operational temperature. The latter effect would be key in reducing operational costs. Likely, the chemisorption energies are increased for all the considered oxides compared to alkaline-earth oxides [1], leading to a reduce vapour pressure, while the ZPE gaps are generally increased for the investigated oxides, thus resulting in higher adsorption selectivities. Selectivity and vapour pressure for V1 of Al_2O_3 are shown in figure 2 and, as expected, exhibit opposite trends. It is noticed that a favorable temperature window can be identified so that both high selectivity and sufficiently high vapor pressure are simultaneously achieved. This range corresponds to experimentally accessible operating conditions, indicating that efficient isotope separation can be realized without requiring extreme conditions.

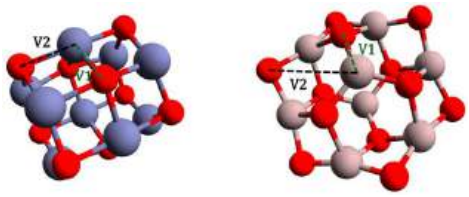

Fig. 1. (left) model for Zn_9O_9 (right) model for M_8O_{12}

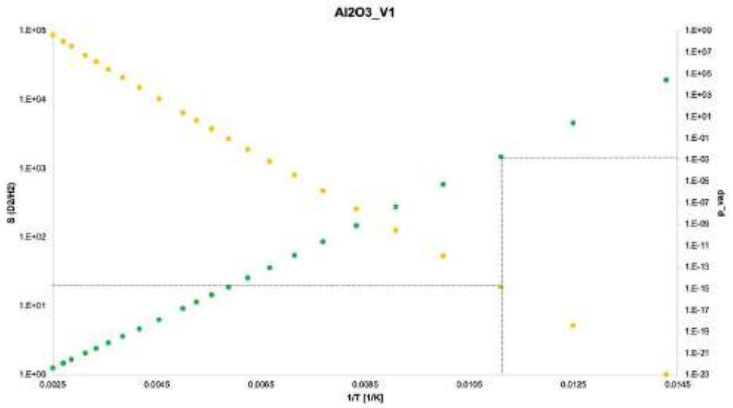

Fig. 2. $S(D_2/H_2)$ and $p_{vap}(H_2)$ from 70 to 400 K for Al_2O_3_V1

[1]Puricelli S.; Bruno, G.; Gatti C.; Ponti A.; Mella M. *Applied Surface Science*, **2024**, 657, 159596.

APC - D4 - O09

X-Ray fluorescence as a novel, flow-through, element-based detector for universal quantification in Liquid Chromatography

Gaëlle Spileers[1], Pieter Tack[2], Laszlo Vincze[3], Frédéric Lynen[1]
[1]Separation Science Group Ghent University, Belgium; [2]Ghent University Centre for Tomography (UGCT), Belgium; [3]X-ray Microspectroscopy and Imaging Group Ghent University, Belgium

Despite the availability of numerous HPLC detectors, few provide a universal, molecule-independent response while maintaining selectivity. This limitation can be addressed through the use of elemental detectors which rely on element-specific calibration curves instead of compound-specific ones, thereby eliminating the need for authentic standards. This feature is especially useful for the analysis of large compound classes, derivatives, degradation and reaction by-products for which standards are often too expensive or entirely unavailable.

Inductively coupled plasma mass spectrometry (ICP-MS) is one such elemental detector. However, it is hindered by hyphenation difficulties, high cost and its destructive nature which inhibits coupling with other detectors. Therefore, X-Ray Fluorescence (XRF) is proposed as a more simple and affordable alternative. Similar to ICP-MS, XRF offers universal quantification through element-specific fluorescence energies with additional advantages such as broad linear range and seamless compatibility with other detectors owing to its flow-through nature.

XRF is commonly employed as a static detector across various disciplines. However, its use is limited in dynamic systems, with hyphenation to capillary electrophoresis scarcely explored and its first use with HPLC in 2025.[1] Theoretically, XRF enables the analysis of elements down to Sodium, however, the primary constraint lies in sensitivity rather than capability. Current detection limits for HPLC-XRF are moderate but they do not appear to be an intrinsic limitation, and substantial improvements are still anticipated. To assess the future potential of HPLC-XRF, the technique was also tested at the European Synchrotron Radiation Facility. The sensitivities achieved with high-intensity X-ray beams provide a good indication of what may be attainable with laboratory-scale sources in the future.

This presentation aims to introduce the concept of HPLC-XRF, outline its current capabilities and state of the art, and provide insights into future development.

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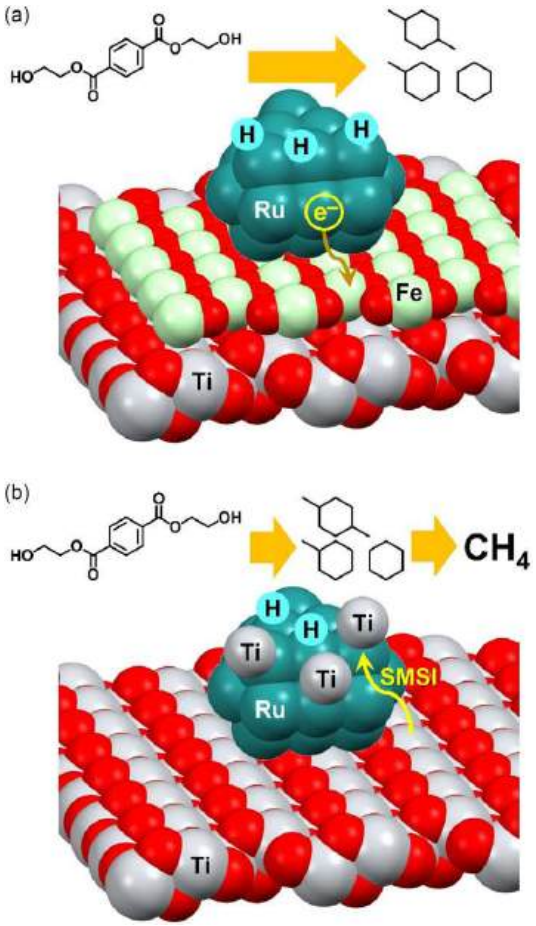
APC - D4 - O10

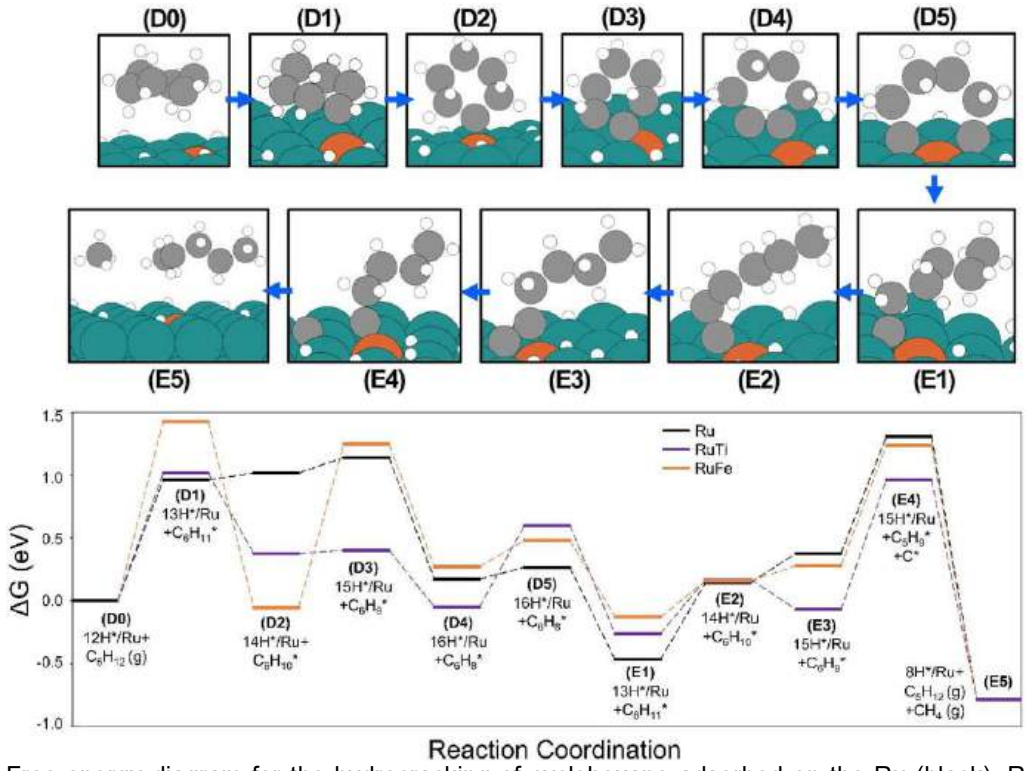
TiO_2-supported Ru–Fe catalysts for the hydrodeoxygenation of bis(2-hydroxyethyl) terephthalate (BHET) prepared by the glycolysis of polyethylene terephthalate (PET)

Jeonghun Kim[1,2], Yerin Lee[1,3], Kangtaek Lee[3], Kyeongsu Kim[1,2], Jeong-Myeong Ha[1,2]
[1]Clean Energy Research Center, Korea Institute of Science and Technology, Republic of Korea; [2]Division of Energy and Environment Technology, KIST School, University of Science and Technology, Republic of Korea; [3]Dept. of Chemical and BiomolecularEngineering, Yonsei University, Republic of Korea

Polyethylene terephthalate (PET) upcycling to petrochemical feedstocks proceeded through catalytic hydrodeoxygenation (HDO) of bis(2-hydroxyethyl) terephthalate (BHET) prepared by glycolysis of PET. TiO_2-supported ruthenium catalysts produced deoxygenated compounds that included aromatic and cyclohexyl molecules. A hydrogen-pressure-dependent deoxygenation pathway was inferred from the detected intermediates. With iron added to Ru/TiO_2 ($Ru/Fe/TiO_2$), the carbon yield to C6–C8 deoxygenated compounds reached 61.1%. Proximity of Ru to Fe oxides depleted the electron density of Ru, adjusted its catalytic activity, and suppressed excessive hydrocracking, which preserved high yields of C6–C7 hydrocarbons. To elucidate the experimental results, we first investigated the chemical state of Fe. Based on XPS data and literature study, iron oxide was modeled as Fe_3O_4[1]. To examine the possibility that Fe_3O_4 suppresses SMSI, the oxygen vacancy formation energy of Fe_3O_4 was calculated. Finally, the mechanism of cyclohexane ring-opening followed by hydrocracking was studied on Ru, RuFe, and RuTi surfaces to investigate how the presence of SMSI influences product distribution[2,3].



Schematic conversion of BHET on (a) $Ru/Fe_x/TiO_2$ and(b) Ru/TiO_2



Free-energy diagram for the hydrocracking of cyclohexane adsorbed on the Ru (black), RuTi (purple), and RuFe (orange) surfaces

Jeonghun Kim and Yerin Lee contributed equally to this study.

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Computational Chemistry & AI: The Power of Data (CAI)

CAI - D1 - O01

Binding energies of sulfur–bearing species on neutral and charged amorphous solid water ices

Irina Grubova[1], Kaat Verhagen[1], Tobe Vorsselmans[1], Erik C. Neyts[1]
[1]Research Group MOSAIC, Dept. of Chemistry, University of Antwerp, Belgium

In the dense and cold regions of molecular clouds, gas–phase sulfur (S) is depleted by two to three orders of magnitude relative to its cosmic abundance. This discrepancy is known as the long–standing S depletion problem. Its disappearance in dense regions suggests efficient removal from the gas phase, potentially through adsorption onto interstellar dust grains coated with amorphous solid water (ASW) ice mantles. Identifying the molecular reservoirs of S in these ices therefore remains a key open question in astrochemistry [1,2].

S–bearing molecules are thought to have played an important role in prebiotic chemistry on early Earth. Recent astronomical observations include the detection of SO_2 in the atmosphere of the exoplanet WASP–39b and S–bearing species such as H_2S, SO_2, OCS, and SO in the coma of comet 67P/Churyumov–Gerasimenko [3]. These findings highlight the need to understand how S is processed and stored in interstellar ices and incorporated into planetary systems.

Under interstellar conditions, surface processes such as adsorption, diffusion, and desorption are governed by the binding energies (BEs) of molecules to the ice. Cosmic radiation and low–energy electrons can induce negative charging of interstellar dust grains. This charging may modify molecule–ice interactions, but its effect remains poorly constrained.

Here, we investigate the BEs of astrochemically relevant S–bearing species on neutral and negatively charged ASW surfaces using DFT calculations. Our results show that negative surface charging generally enhances the BE of S–bearing species, although this effect is species dependent. These findings provide new constraints for astrochemical models and contribute to a better understanding of S sequestration in dense molecular clouds.

This work was supported by the MSCA Fellowship (No. 101211724).

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CAI - D1 - O02

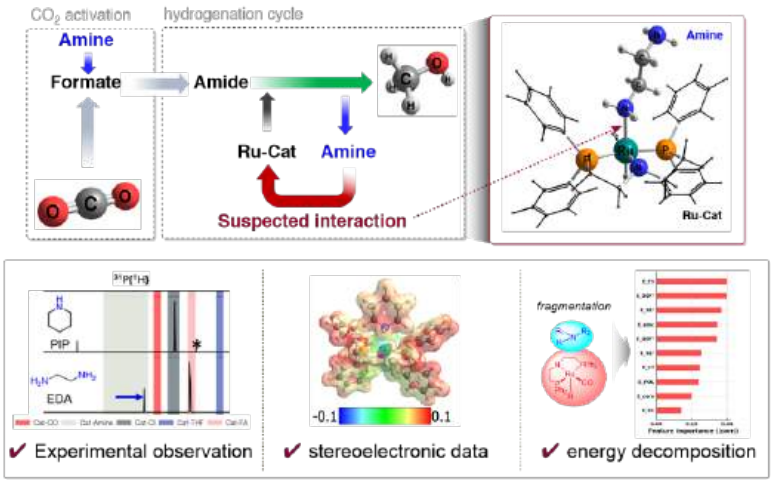
Uncovering the origin of amine-driven selectivity in Ru-catalyzed CO_2-to-methanol hydrogenation

Muhammad Dzulfahmi Ramadhan[1,2], Damdae Park[1], Jinwoo Choi[3], Jaehyeong Choi[1], Ung Lee[1,2,a], Jong Suk Yoo[3,a], Kyeongsu Kim[1,2,a]

[1]Clean Energy Research Center, Korean Institute of Science and Technology, Seoul, Republic of Korea; [2]Division of Energy & Environment Technology, KIST School, University of Science and Technology, Seoul, Republic of Korea; [2]Dept. of Chemical Engineering, University of Seoul, Seoul, Republic of Korea

Amine-assisted CO_2 capture and conversion has emerged as a promising router for methanol synthesis, yet experimental studies consistently demonstrate that amine identity strongly governs selectivity between formamide and methanol formation.[1, 2] Despite extensive investigation, this selectivity cannot be universally rationalized using conventional descriptor such as amine basicity or pKa. Likewise, density functional theory (DFT) analyses focused on reaction energies along the reaction along the hydrogenation pathway is not adequate to explain the observed divergence in catalytic outcomes.[3] Here, we elucidate the origin of selectivity in Ru-catalyzed CO_2 hydrogenation is controlled by amine behavior towards catalyst resting state which can either act inhibitively to limit the hydrogenation cycle by forming amine-catalyst complex, or assistively by facilitating catalyst reactivation via dihydrogen cleavage. Experimental observation reveals characteristic of hydride signatures of direct amine-catalyst interactions under the NMR measurements, suggesting that certain amines potentially trap the active catalyst.

A diverse set of amine candidates was evaluated both experimentally and computationally for their selective conversion to methanol. Energy profiles obtained from DFT calculation along two distinct pathways of catalyst reactivation were collected along as the experimental data. Decision tree analysis then being conuducted to identify key intermediates governing catalytic outcomes, with the Wiberg bond index (WBI) of the amine-catalyst addut (**2A** state) emerging as the primary descriptor. Subsequent stereoelectronic and fragmentation analysis including natural bond orbital (NBO) and natural energy decomposition analysis (NEDA), provide mechanistic insight into the electronic origin of amine-dependent selectivity. Together, these results establish amine-catalyst adduct formation as a central mechanistic factor controlling methanol production in Ru-catalyzed CO_2 hydrogenation.



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CAI - D1 – O03

New computational insights into the speciation and formation of polyoxometalates

Carles Bo[1,2*], Jordi Buils[1,2], Diego Garay-Ruiz[1], Laura S. Junkers[2], Enric Petrus[2],Mireia Segado-Centelles[2]
[1]Institute of Chemical Research of Catalonia (ICIQ), Spain; *[2]Dept. de Química Física I Inorgànica, Universitat Rovira i Virgili, Spain*

In recent years our group has been working in the development of a new computational methodology, which we called POMSimulator,[1] to simulate the complex multi-species multi-equilibria taking place in the self-assembly processes leading to polyoxometalates. POMSimulator comprises automated workflows that rely exclusively on DFT-based results, and has been successfully applied to Mo, W, V, Nb and Ta isopolyoxometalates (IPAs). [2,3] The reaction networks discovered automatically can be applied to perform very long multi-time scale kinetic simulations on the formation of isopolyoxotungstanates, [4] what led to the discovery of a reaction mechanisms. We released recently the first open-source version of the code. [5] On the other hand, heteropolyoxoanions (HPAs) introduce far more complexity. We carried out a statistical analysis of the massive amounts of data produced by POMSimulator to reduce the reliance of the method on experimental formation constants. [6,7] More recently, we combined the predictions of our method with new X-Ray total scattering data to investigate polyoxomolibdates speciation under hydrothermal conditions.[8] A summary of all these discoveries plus new recent computational experiments will be presented.

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CAI - D1 - O04

Modelling singlet oxygen generation on Ru-functionalized metal organic frameworks with trapped ion quantum computers

Carlo Alberto Gaggioli[1], David Zsolt Manrique[1], Gabriel Greene-Diniz[1], Connor Lenihan[1], Kripa Panchagnula[1], Luca Erhart[1], Gabriel Laude[1], Thomas Soini[1], Elvira Shishenina[1], David Muñoz-Ramo[1]
[1]Quantinuum, UK

Metal-Organic Frameworks (MOFs) have recently shown the ability to produce singlet oxygen with potential use in photodynamic therapy (PDT). We have studied the rate of singlet oxygen generation on a ruthenium functionalized MOF (DBB-Ru)[1] by means of Density Functional Theory (DFT). DFT calculations yield a wide range of values, owing to the sensitivity of excited state energies to the functional used. In order to get more precise estimations on the energies needed to calculate the rate, we turn to active space methods together with quantum computations. By employing novel energy estimators, we demonstrate the capability of Quantinuum's newest trapped-ion device Helios[2] for large qubit counts and reduced shot counts. The combination of state-of-the-art hardware and algorithms enabled the calculations of excited state energies with high precision for active spaces of up to 10 electrons in 10 orbitals, setting the path to scalability to larger active spaces and revealing the predictive power of current and future quantum computing hardware for complex chemical simulations.

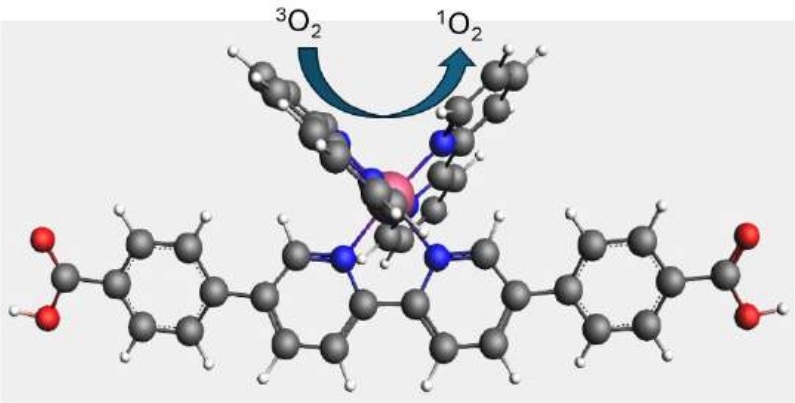

Fig. 1. Scheme of the singlet oxygen generation on the linker of the DBB-Ru MOF.

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CAI - D1 - O05
Multiscale computational insights into thermal and catalytic pyrolysis of polyolefins

Feixiang Xu[1], Eelco Vogt[1], Bert Weckhuysen[1]
[1]Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Dept. of Chemistry, Utrecht University, The Netherlands

With global plastic consumption continuing to rise, the high-value chemical recycling of waste plastics has become an urgent research priority. Thermal and catalytic pyrolysis offer promising pathways to convert plastic waste into valuable chemicals and fuels, where hydrogen-transfer and β-scission reactions govern product distributions. However, the microscopic mechanisms underlying these cracking pathways remain difficult to probe experimentally, and conventional static density functional theory (DFT) methods fail to capture the substantial conformational fluctuations and anharmonic effects that dominate high-temperature bond activation. To overcome these limitations, we developed a multiscale computational framework to resolve the atomic-level behavior of polyolefins during both thermal and catalytic pyrolysis. The first step is to employ Ab initio molecular dynamics (AIMD) to capture high-temperature decomposition dynamics and to sample reactive conformations along the anharmonic free-energy landscape. These structures are subsequently refined using DFT to identify transition states and quantify reaction barriers, revealing how conformational excitations mediate key reaction steps. Because AIMD is computationally prohibitive for large polymer–catalyst systems, reactive force field molecular dynamics (ReaxFF MD) is used to explore catalytic pyrolysis over extended length and time scales. To address the limited accuracy of existing force fields, DFT-derived data are used to train a highly accurate reactive potential force field capable of reliably describing C–C scission, hydrogen transfer, and catalyst-induced reaction pathways[1]. By integrating AIMD, DFT, and machine-learned reactive force fields (MLFFs), this study reconstructs a reactive potential energy surface for polyolefin pyrolysis and provides a comprehensive microscopic picture of both thermal and catalytic cracking. The resulting framework offers fundamental insights into pyrolysis reaction mechanisms and serves as a powerful tool for the rational design of catalysts for high-value plastic waste upcycling.

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CAI - D1 - O06

Carbonate-radical pathway in dual nickel/carbon nitride photocatalysis: A new mechanistic blueprint for C(sp^3)-H activation

Elisabetta Inico[1], Miguel M. de Vries Ibáñez[1], Carlo Alessandro Cavallotti[1], Gianvito Vilé[1]
[1]Dept. of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Italy

The selective functionalization of C(sp^3)-H bonds is a key step in modern synthesis, allowing access to complex fine chemicals. While visible-light dual photocatalysis has enabled significant progress, prevailing mechanistic models, notably invoking halogen-radical (Br·) intermediates, fail to rationalize key experimental observations, including base dependence and regioselectivity. Here, we present a theoretical mechanistic study, supported by experimental evidence, of a visible-light-driven nickel/carbon nitride (CN_x) dual catalytic system for direct C(sp^3)-H functionalization (Figure 1a). All DFT calculations were performed with Gaussian 16 using the rev-DSDPBEP86 and PBE0-D3 functionals. Our calculations reveal that the reaction proceeds through a previously unrecognized base-activated pathway that decisively rules out the classical Br·-mediated mechanism.[1-2] Specifically, upon photoactivation, CN_x is photoexcited to its triplet state, which initiates the catalytic cycle, promoting single-electron transfer from the base, generating a $CO_3^{\cdot-}$ radical anion that activates THF (Figure 1b). Free energy surface analysis (Figure 1c) shows that carbonate oxidation and hydrogen abstraction from the C-H donor are both thermodynamically and kinetically favorable, explaining the experimentally observed base requirement and excluding a direct hydrogen atom transfer pathway. The resulting THF· radical is captured by the nickel catalytic cycle, following oxidative addition of the aryl bromide. Radical interception at Ni^{II} affords Ni^{III} intermediates, which undergo low-barrier C-C bond-forming, releasing the product. Electron transfer from reduced CN_x regenerates both catalysts, closing the coupled dual catalytic cycles. Spectroscopic experimental evidences support these theoretical results. Overall, this work redefines the mechanistic landscape of carbon nitride-mediated dual photocatalysis, introducing a carbonate-radical-driven C(sp^3)-H activation paradigm, and provides a general framework to rationalize base effects, regioselectivity, and substrate reactivity in sustainable C-H functionalization under visible light.

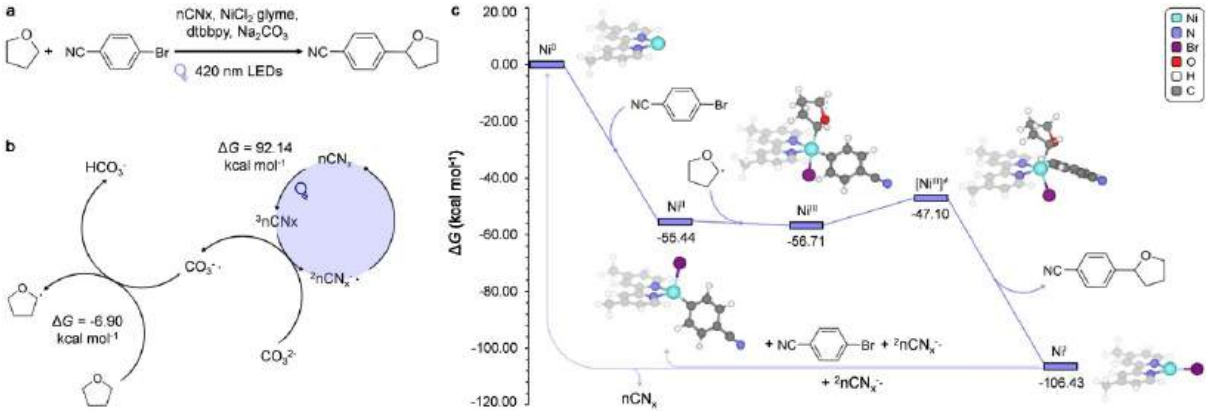

Fig. 1. Catalysing carbon nitride and nickel complexes for C-H activation in C(sp^2/sp^3)-C(sp^3) cross-coupling reaction (a). In panel (b) and (c), the mechanism and calculated free energies are reported, respectively.

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CAI - D1 - O07
PyOrbb - Automated analysis tool for orbital interactions

Yuman Hordijk[1], Steven E. Beutick[1], Xiaobo Sun[1,2], Laurens Groot[1], Tori Gijzen[1], Jordi Poater[2,3], Trevor A. Hamlin[1], F. Matthias Bickelhaupt*[1,4,5], Célia Fonseca Guerra*[1]
[1]Dept. of Chemistry and Pharmaceutical Sciences, Amsterdam Institute of Molecular and Life Sciences (AIMMS), Vrije Universiteit Amsterdam, The Netherlands; [2]Dept. de Química Inorgànica i Orgànica & IQTCUB, Universitat de Barcelona, Spain; [3]ICREA, Spain; [4]Institute of Molecules and Materials, Radboud University, The Netherlands; [5]Dept. of Chemical Sciences, University of Johannesburg, South Africa

We present PyOrbb, an open-source, user-friendly Python-based program that automates the analysis and visualization of orbital interaction mechanisms between molecular fragments or reactants, based on quantum-chemical computations performed with the Amsterdam Density Functional (ADF) program. Using a novel orbital interaction detection algorithm, PyOrbb extracts essential mixing patterns, presents them in an interactively adjustable orbital interaction diagram, and summarizes all relevant quantitative data in a convenient Excel spreadsheet for further analysis. The tool enables efficient interpretation of chemical bonding across a broad range of systems, including challenging examples from organic, inorganic, and supramolecular chemistry. PyOrbb is shown to accurately and instantaneously visualize relevant bonding mechanisms from the often overwhelming output of density functional computations. We will explain in detail the novel algorithm we devised to identify and rank orbital interactions and demonstrate PyOrbb's ability to analyze molecular systems of practical chemical interest, both strongly and weakly bound.

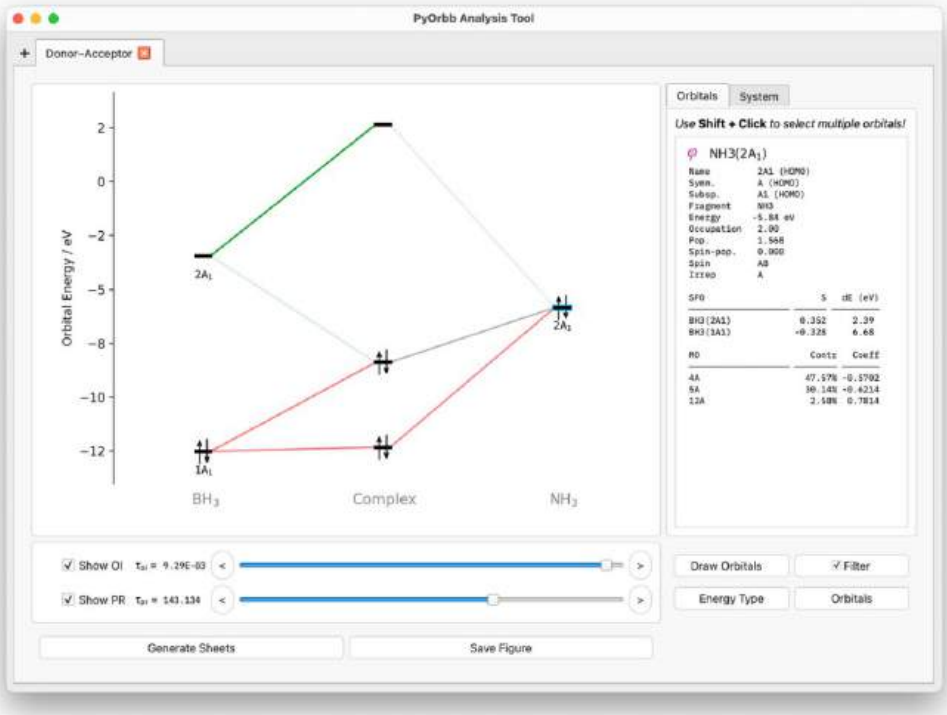


Fig. 1. The PyOrbb graphical user interface used to analyze the formation of the $NH_3 \rightarrow BH_3$ Lewis pair.

Fig. 2. The PyOrbb logo.

Acknowledgments and Funding: We thank Marco Dalla Tiezza for helpful discussions, and the Chinese Scholarship Council (CSC), the Spanish MINECO (CTQ2016-77558-R and MDM-2017-0767), the Generalitat de Catalunya (2017SGR348), the Netherlands Organization for Scientific Research (NWO), and Microsoft Research for financial support. This work was supported by Open Life Science (OLS) as part of its (Open Seeds/Nebula) training programme.

CAI - D1 – O08

Understanding the Raman spectra of silica prenucleation clusters via ab initio molecular dynamics and experiments

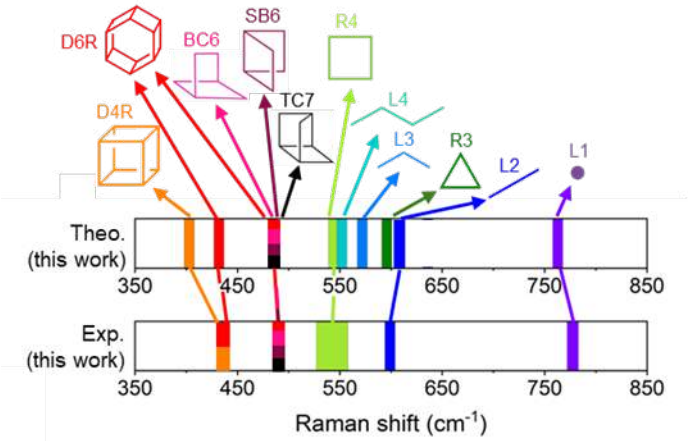
Fileto Rodríguez[1], Ionut Tranca[1], Pablo Beato[2], Monica Calatayud[3], Frederik Tielens[1]
[1]Vrije University Brussel, Belgium; [2]TOPSOE A/S, Denmark; [3]Sorbonne Université, France

Silica's speciation has proved to be a complex phenomenon with far-reaching implications. Techniques capable of characterizing silica oligomers are paramount due to the diversity of applications involved, from functional additives to the non-classical nucleation routes of silica-based materials. ^{29}Si NMR remains the most successful technique for the characterization of silica's speciation. However, its limited applicability beyond research underscores the need for a powerful, sustainable and versatile alternative with *in situ* characterization potential.[1] Raman spectroscopy has proven its potential to fulfill these requirements.

In this work, we tackled a decades-old challenge: the unique assignment of Raman features in silica oligomers. Integrating experimental Raman measurements with state-of-the-art ab initio dynamic Raman simulations and conformationally averaged static DFT calculations, we deconvolute the complex vibrational response of silica-containing solutions. Our approach explicitly incorporates largely overlooked theoretical contributions, such as anharmonicity, realistic solvation, and conformational diversity, enabling robust assignments of Raman bands to individual species.[2]

Moreover, using the same integrated approach, we complete the database of Raman signals for most of silica oligomers, allowing for the discovery and rationalization of the underlying trends in their spectra.[3] Furthermore, we address the effect of protonation in the spectra, and the common use of inappropriate notations to describe the vibrations of such oligomers.

Bringing Raman spectroscopy into the toolbox for the determination of silica's speciation offers two key advances. First, real-time *in situ* characterization can significantly deepen our understanding of nucleation and growth pathways in silica-based systems. Second, improved control over synthesis enables the development of more sustainable synthetic protocols, by reducing waste associated with unwanted by-products, while accelerating the discovery of novel materials with promising functional properties.



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CAI - D1 - O09
Molecular aggregation and microheterogeneity in various aqueous solutions

Ravi Singh[1], Jonghyuk Ryu[1], Jun-Ho Choi[1]
[1]Dept. of Chemistry, Gwangju Institute of Science and Technology (GIST), Republic of Korea

Recently, we propose a relationship between molecular aggregation pathway and physical properties of aqueous solutions in diverse binary systems, including ions, alcohol, osmolytes and so on.[1] That is, closely packed aggregates tend to be separated from liquid water by minimizing interaction with water, whereas spatially extended aggregates are completely miscible by fully interacting with water. Conducting combination study of molecular dynamics (MD) simulation, graph theory and spatial distribution analysis, it is shown that this bifurcating aggregation behavior generates distinct spatial distribution of constituent molecules,[2] and modulates water H-bond structure and eventually solubility and phase behavior in various binary mixture systems.[3] In the case of osmolyte solutions, trimethylamine-N-oxide (TMAO) as a protecting osmolyte shows a tendency to remain isolated with less formation of osmolyte aggregates whereas there is a strong aggregation tendency in the denaturant tetramethylurea (TMU) solution, due to favored hydrophobic interactions between TMU molecules. This comprehensive studies in aqueous osmolyte solutions revealed how water structure and dynamics are modulated in the presence of osmolyte aggregates and how the aggregation behavior dictates the mode of osmolyte action.[4]

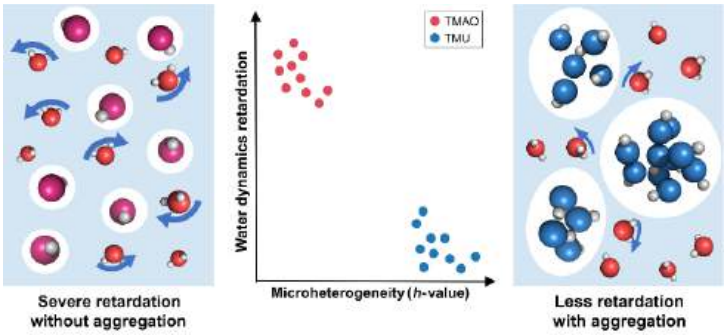

Fig. 1. Water dynamics under distinct microheterogeneity of aqueous osmolyte solutions. The water motions are significantly retarded when the solute molecules are evenly dispersed. In contrast, the water dynamics is less disturbed in the presence of osmolyte aggregates. The microheterogeneity is quantified by a theoretical index of the *h*-factor.

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CAI - D1 - O10

CYtochrome complex ligand optimization with protein simulation – An automated pipeline for simulations and analysis of CYP450 docked structures

Przemysław Grenda[1], Martyna Ogos[1,2], Eugen Hruška[1]
[1]Dept. of Biophysics and Physical Chemistry, Faculty of Pharmacy, Charles University, Czech Republic;
[2]Dept. of Physicochemical Drug Analysis, Faculty of Pharmacy, Jagiellonian University Medical College, Poland

Although molecular docking is computationally efficient, it frequently lacks the structural precision necessary for accurate binding mode prediction—a limitation mitigated by molecular dynamics (MD) equilibration.[1] However, high-throughput MD automation remains a challenge, particularly for complex systems involving covalently bound cofactors.

To bridge this gap, we introduce CYCLOPS[2], a Python-based automated pipeline built on the OpenMM engine. This workflow seamlessly integrates ligand and heme parameterization, enabling the GPU-accelerated refinement of complexes generated via both rigid and flexible docking protocols. In validation benchmarks, the automated setup achieved a high success rate for rigid docking inputs (~85%), whereas RoseTTAFold All-Atom structures exhibited lower compatibility (~50%) primarily due to ligand stereochemical artifacts. By streamlining these processes, CYCLOPS significantly lowers the barrier for large-scale MD refinement of cytochrome P450 complexes. Finally, the package includes automated analysis modules that aggregate structural and pharmacophoric trajectories to facilitate direct comparison with experimental observables. This enables a robust statistical assessment of the generated conformational ensembles and validates the applicability of MD to docked cytochrome P450 structures.

Authors acknowledge funding by Charles University and Faculty of Pharmacy, Charles University through grants No. PRIMUS/24/MED/004, UNCE/24/MED/008, and SVV 260 663.

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CAI - D1 - O11
Computational engineering of peptides inhibiting cell death

Tom Vlaar[1], Bernadette Mayer[1], Jonathan Kunz[1], Lars van der Heide[2], Ioana M. Ilie[1]
[1]van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands; [2]Swammerdam Institute for Life Sciences, University of Amsterdam, The Netherlands

The proteins of the Bcl-2 family play crucial roles in regulating apoptosis. It is divided into pro-survival and pro-apoptotic proteins that determine cellular fate. In particular, Bax is a crucial executor of apoptosis as its activation initiates the apoptotic phenotype. Hence, targeting this protein represents an attractive therapeutic approach, which can aid in regulating apoptotic signalling and potentially contribute to the development of novel therapies against cancer and neurodegenerative diseases.
Here, we introduce a digital paradigm, which relies on rational design, artificial intelligence and computer simulations to develop and validate peptide-based agents that bind to Bax, thereby inhibiting its apoptotic properties[1,2]. The peptides are designed and optimized to bind to Bax starting from the crystal structures of affimers in a complex with Bcl-2 proteins. Next, molecular dynamics (MD) simulations are employed to probe the stability of the Bax–peptide complexes and to estimate the binding free energies.
The results show that the designed peptides bind with high affinity to Bax. The designed peptides bind in the canonical hydrophobic groove (BH1 domain) of Bax and are experimentally validated. Notably, the peptides restrict the flexibility of the α1–α2 loop, modulating the trigger bottom site associated with toxicity. All in all, the results highlight the potential of these peptides as valuable tools for further exploration in modulating apoptotic pathways.

CAI - D1 - O12

The sampling-based adaptive biasing force (sABF) method efficiently explores the free energy landscape of large-scale motions in liquid-phase systems

Dieu Hang Tran[1], Jordy Peeters [1], Kenno Vanommeslaeghe[1]
[1]Dept. of Analytical Chemistry, Applied Chemometrics and Molecular Modelling (FABI), Vrije Universiteit Brussel (VUB), Belgium

Adaptive Biasing Force (ABF) is a popular free energy method for studying motions in condensed-phase systems along a specific set of Collective Variables (CVs).[1][2] While it is conceptually simple and easy to set up, applying ABF in its most basic form to real-life biomolecular problems often yields poor convergence because the CVs tend to span relatively long distances. This gave rise to more sophisticated ABF-based methodologies that partially mitigate this problem, at the cost of ABF's simplicity. In essence, applying an ABF-based method on a large motion in a biomolecule requires significant pre-existing knowledge and insight.
We briefly discuss how the Einstein–Smoluchowski relation (also known in its more generalized form as the fluctuation-dissipation theorem) becomes a fundamental source of hysteresis when using an external force to drive displacements with amplitudes of more than a few atoms in liquid-phase systems. While the convergence of the original ABF method is particularly vulnerable to this phenomenon, we show how our sABF implementation addresses this problem. This results in relatively fast-converging Potentials of Mean Force of large motions in biomolecules, which is demonstrated using two transmembrane proteins as examples. Compared to other advanced ABF variants, the sABF method is easy to use and automate because it has no parameters in addition to the ones already present in the most basic ABF implementation.

The supercomputing resources and services used in this work were provided by the VUB and the VSC (Flemish Supercomputer Center), the latter being funded by the FWO and the Flemish Government, through project 2023_100.

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CAI - D1 - O13
Higher accuracy reaction rates with the ab initio nanoreactor

Eugen Hruška[1], Fang Liu[2]
[1]Dept. of Biophysics and Physical Chemistry, Faculty of Pharmacy, Charles University, Czech Republic;
[2]Dept. of Chemistry, Emory University, USA

Our understanding of chemical reaction rates is impeded by limitations of contemporary computational methods for reaction rate constant estimation. An alternative to transition state optimization approaches is the ab initio nanoreactor, which allows the automated ab initio discovery of larger reaction networks with limited a priori information.[1]
In this work, we modify the ab initio nanoreactor setup and the chemical reaction event detection algorithm. This approach improves the accuracy of the estimated reaction rate constants, and allows to estimate the uncertainties for these estimates. We demonstrate the improved capabilities on high-temperature reactions involving sulfur, where we estimate a reaction network at DFT accuracy containing hundreds of reactions. The joint estimation of reaction rate constants and their uncertainties allowed us to evaluate the applicability domain for the estimated chemical reaction network. Due to the aforementioned improvements, the applicability domain has been extended.

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CAI - D1 - O14

Bridging molecular dynamics and COSMO-RS simulations with macroscale modeling for advancements in polyurethane post depolymerization separation processes

Christophe de Graaf[1], Pieter Billen[1], Philippe Nimmegeers[2,3,4], Remco W.A. Havenith[5,6], Ana V. Cunha[7]
[1]Faculty of Applied Engineering, Intelligence in Processes, Advanced Catalysts and Solvents, University of Antwerp, Belgium; [2]Dept.of Engineering Management, Faculty of Business and Economics, University of Antwerp, Belgium; [3]Flanders Make@UAntwerp, Belgium; [4]NANOlight Centre of Excellence, Belgium; [5]Stratingh Institute for Chemistry, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands; [6]Ghent Quantum Chemistry Group, Dept. of Chemistry, Ghent University, Belgium; [7]National Center for Computational Sciences, Oak Ridge National Laboratory, USA

Polyurethane (PU) is a versatile and widely used polymer made from polyols and isocyanates. It is valued for its durability, flexibility, and thermal insulation properties, which has led to extensive applications in furniture, construction insulation, automotive components, coatings, and adhesives. However, the same chemical stability and cross-linked structure that make PU performance-efficient also render it difficult to recycle through conventional mechanical or chemical methods. As a result, PU waste represents a growing environmental challenge, accumulating in landfills where it can persist for decades, contribute to microplastic pollution, and increase reliance on incineration, which may release hazardous emissions. This work presents a workflow to predict separation of polyols and isocyanate derivatives after polyurethane depolymerization. The workflow encompasses molecular dynamics simulations using the AMBER all-atom force field[1,2] DFT calculations (including tight-binding variants)[3,4] and COSMO-RS[5] calculations to generate a robust database of thermophysical properties required for the NRTL-RK thermodynamic model implemented in ASPEN Plus software[6]. The multiscale nature of the workflow enables consistent information transfer from the molecular to the process level. Results obtained for representative model mixtures show strong agreement with experimental data for polyol extraction, accurately predicting both purity and recovery when compared to laboratory-scale experiments[7], with relative errors lower than 1%. For the isocyanate-derivative fraction, the predicted recovery also agrees well with experimental observations; however, the predicted purity exhibits a deviation of approximately 12%. This discrepancy is attributed to the limited chemical complexity of the current model mixtures, which do not yet fully capture the diversity of species present in real depolymerization streams. Overall, these results demonstrate that computational simulations can play a crucial role in polyurethane recycling by enabling rapid screening of polymer formulations, depolymerization pathways, catalysts, solvents, and operating conditions to identify high-yield, low-energy, and scalable process designs.

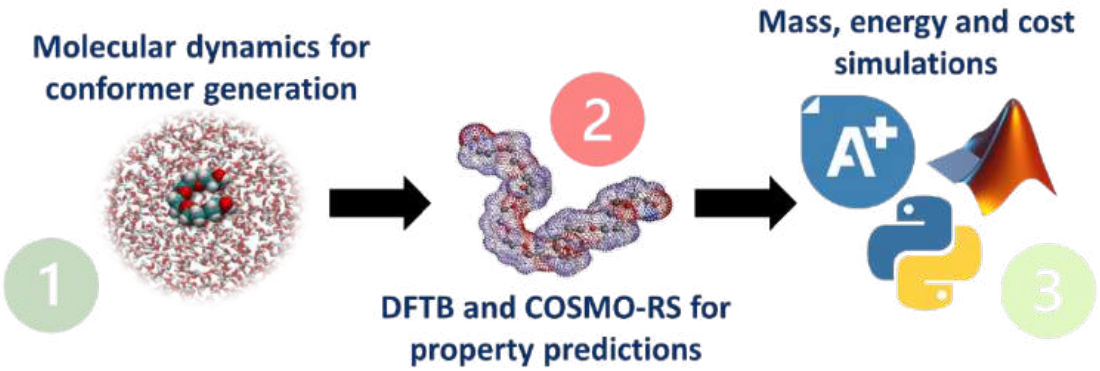

Fig. 1. Workflow for bridging the molecular and macroscale.

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CAI - D1 - O15
Modeling charge transport in radical-containing polymers for all-organic batteries

Anna S. Bondarenko[1], Daniel Escudero[1]
[1]Dept. of Chemistry, KU Leuven, Belgium

All-organic batteries offer a promising solution to metal supply constraints and environmental concerns associated with conventional battery technologies. In this context, radical-containing polymers (RAPs) have emerged as a promising class of materials for all-organic solid-state battery applications. Charge transport in these systems occurs via hopping of electrons between pendant radical groups. However, a detailed understanding of charge transport mechanisms is lacking, hindering our ability to design these materials from the bottom up.
Here, we develop a multiscale model combining realistic atomistic-level structures with accurate quantum dynamical modeling of charge transport. The model enables the simulation of polymer morphologies that are validated by comparing thermophysical properties to experimental data. Microscopic electronic parameters—such as energy levels, electronic couplings, and electrostatic embedding—are then obtained and fed into the quantum dynamical modeling, allowing for an embedded modeling of charge transport in these materials. We compare a well-studied cathode material with the polymer that has the record electronic conductivity for this class of materials to date.

A.S.B. acknowledges the support from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie (grant No. 101210559).

CAI - D1 - O16
Catch the heat: In porous and non-porous materials

Ionut Tranca[1], Aleksandr Shkatulov[2], Veerapandian Ponnuchamy[1], Dimitrios Sakellariou[3], Indy Boumon[1], Mohamed Sherif[4], Silvia Nedea[4], Emre Genc[5], Hilal Kucuk[5], Frederik Tielens[1]
[1]Vrije Universiteit Brussel, Belgium; [2]The Iberian Energy Storage Research Center, Spain; [3]Katholieke Universiteit Leuven, Belgium; [4]Eindhoven University of Technology, Netherlands; [5]Gazi University, Turkiye;

In order to tackle the modern challenges of climate change, resources depletion and geopolitical instability, the human society will have to evolve towards sustainable energy and green economy. Energy storage will play a paramount role in this global energy system, in order to support the penetration of the fluctuating renewable energy sources (sun, wind), as well as to capture the waste from various domestic or industrial processes.
As of 2022 **heat is the world's largest energy end-use**, accounting for ~50% of the world energy consumption (more than electricity-30% or transport-20%). About half of this heat is used in domestic applications, with the other half being used in industry. Creating efficient heat batteries able to store renewable and waste heat from natural (Sun) or artificial (industry) sources, at various temperatures, will be crucial for the implementation of the sustainable energy systems of the future.
Thermochemical energy storage (TCES) through reversible chemical reactions (sorption/desorption of gases like H_2O or CO_2) is the most promising technology for compact and lossless long-term heat storage. The current research in this field is hampered by the scarcity of appropriate TCES materials that can store and release heat at the desired temperatures with high efficiency and storage density. Thus, novel promising candidates are required, along with means of screening the large potential chemistry structural space.
In our work we performed a high-throughput screening of structural databases (COD, ICSD, hMOF, CoreMOF) and by using a combination between machine learning, GCMC / MD / DFT-calculations and advance chemical reactivity descriptors we explore both porous (MOFs) and non-porous (salt hydrates, metal oxides) materials relevant for heat storage at low and high temperatures. For MOFs a toolkit to assist researchers and engineers in materials discovery is developed.

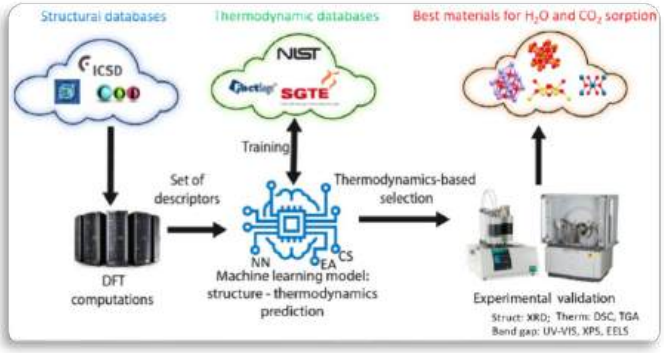

Fig.1. Screening salts and oxides for thermochemical heat storage

Fig. 2. EvoMOF – a tool for screening and designing (in the future) MOFs.

CAI - D1 - O17
Harnessing noncovalent interactions from catalysis to quantum technologies

Lorenzo Baldinelli[1], Filippo De Angelis[1,2,3], Giovanni Bistoni[1]
[1]Dept. of Chemistry, Biology and Biotechnology, University of Perugia, Italy; [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di Scienze e Tecnologie Chimiche "Giulio Natta" (CNR-SCITEC), Italy; [3]SKKU Institute of Energy Science and Technology (SIEST), Sungkyunkwan University, Korea

In this talk, we present a computational analysis of how noncovalent interactions can be quantified and exploited to control chemical behavior across different molecular systems (Figure 1).[1]
Representative examples span asymmetric catalysis[2,3] and molecular qubits.[4] In confined chiral catalytic environments, noncovalent interactions shape conformational landscapes and stabilize competing transition states, thereby directly influencing reaction selectivity. In molecular qubits, interactions with the surrounding host matrix modify their spin structure, enabling control over properties relevant to information storage and robustness without modifying the qubit itself.
Although these systems differ widely in nature and application, they share a common underlying principle: chemical function is encoded in the collective balance of noncovalent interactions rather than in any single isolated force. By adopting an interaction-centric computational framework, this work provides a coherent picture that connects electronic structure to function across length scales, offering transferable insight for the rational design of functional molecules and materials.

We acknowledge support from UMbriaTECH (Umbria Materials TECHnology District) – CUP: E67G23000220001.

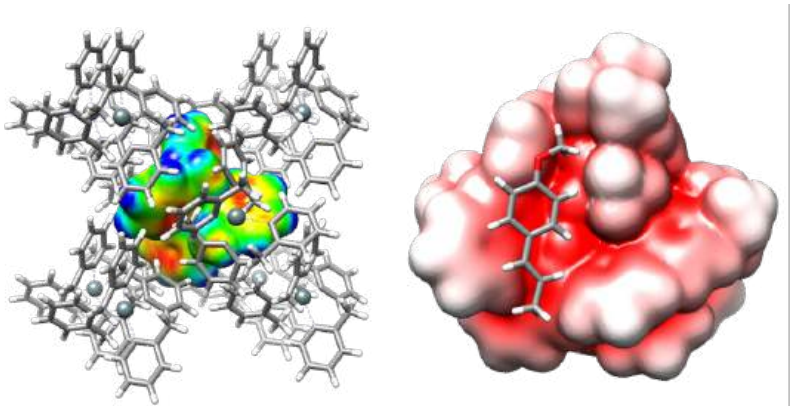

Fig. 1. Left: molecular electrostatic potential (MEP) highlighting matrix-induced electrostatic effects in a molecular qubit.[4] Right: molecular dispersion potential (MDP) illustrating the spatial localization of dispersion interactions within the chiral pocket of an IDPi catalyst.[2]

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CAI - D1 - O18
StereoMolGraph: Reliable computational toolkit for chiral molecules and reactions

Maxim Papusha[1], Kai Leonhard[1]
[1]Institute of Technical Thermodynamics, RWTH Aachen, Germany

A central challenge in chemistry is the faithful representation of molecular structure in a form that enables reliable comparison, classification, and prediction of reactivity. While graph-based molecular representations are widely used, a consistent treatment of stereochemistry remains difficult, particularly for non-tetrahedral stereogenic units and the diverse coordination geometries found in transition-metal complexes. Current cheminformatics standards often rely on specialized or trained descriptors that require manual curation, limiting transferability across different classes of chemical systems.
We introduce a general graph-based molecular representation that encodes stereochemical information through local stereodescriptors grounded in a group-theoretical description of rotational symmetries of atomic environments. This approach provides a unified description of classical tetrahedral stereocenters as well as square-planar, octahedral, and trigonal-bipyramidal coordination geometries within a single extensible framework. By incorporating stereochemistry conservation as an intrinsic graph property, chiral and highly symmetric molecules can be consistently identified and compared using a stereochemistry-aware graph isomorphism algorithm.
Transition states often exhibit fleeting stereochemistry, where stereochemical configurations arise only along a reaction pathway and both reactants and products may be achiral. This behaviour is captured using condensed-reaction-graphs, enabling systematic identification of stereochemically distinct reaction pathways. This is essential for obtaining correct entropic barriers in chemical kinetics.[1]
The stereochemically enriched graph data structures are constructed directly from Cartesian coordinates obtained in quantum-chemical calculations. For practical integration into existing workflows, they are accessible through coordinate-based graph construction as well as bidirectional interfaces to state-of-the-art cheminformatics toolkits such as RDKit.
The methodology is implemented in the Python library StereoMolGraph,[2] providing a practical and extensible foundation for stereochemistry-aware analysis in computational chemistry and enabling chemically consistent interpretation of complex molecular and reaction landscapes.

We acknowledge support of Covestro Deutschland AG and the Werner Siemens Foundation in the frame of the WSS Research Centre "catalaix".

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CAI - D1 - O19

Computationally assisted analysis of CO_2 adsorption in nitrogen-nitrogen linked porous organic polymers

Ivan Kodrin[1]
[1]University of Zagreb Faculty of Science, Dept. of Chemistry, Croatia

Azo-linked porous organic polymers (POPs) are attractive candidates for post-combustion CO_2 capture owing to their nitrogen-rich backbones, which create CO_2-philic microenvironments while retaining synthetic modularity. Nitrogen-nitrogen linkages (azo, azoxy, and azodioxy) offer additional control over CO_2 affinity, but rational optimization is hindered by limited structural information in largely amorphous materials.[1-4] We implement a hierarchical workflow that translates the expected connectivity of a given synthetic route into structures we can model. First, fragment-level calculations are used to rank binding preferences and electrostatic features of nitrogen-nitrogen motifs and key functional groups. Next, the resulting motifs are assembled into idealized 2D layers and evaluated across multiple stacking arrangements. Finally, periodic DFT and electrostatic potential (ESP) mapping, coupled with grand canonical Monte Carlo (GCMC) simulations, are used to predict CO_2 adsorption isotherms, adsorption enthalpies, and adsorption density maps. This approach identifies preferred CO_2 adsorption sites and shows that stacking offsets and site accessibility can dominate performance even when surface areas are comparable. Across trigonal and tetragonal nodes, the simulations rationalize experimental trends and indicate when azoxy and azodioxy nitrogen-nitrogen linkages are expected to enhance CO_2 binding relative to azo analogues. Overall, the workflow provides practical design guidelines that connect linkage polarity and layer stacking to CO_2-framework interactions, supporting informed selection of building units and nitrogen-nitrogen linkages across related POP families.

This work has been fully supported by Croatian Science Foundation under the project IP-2020-02-4467.

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MDR – D1 – O20

Replica Exchange with Flexible Timing (REFT): a novel replica exchange variant for efficient conformational sampling and free energy calculations

Fardine Ameli, Yvan Vander Heyden, Debby Mangelings, Kenno Vanommeslaeghe
Vrije Universiteit Brussel (VUB), Faculty of Medicine and Pharmacy, Research group Analytical Chemistry, Applied Chemometrics and Molecular Modelling, Brussels, Belgium.

Molecular dynamics (MD) simulations are routinely used to study the atomistic behavior of molecular systems. Unfortunately, conventional MD simulations often struggle to sample the full conformational space associated with the process of interest, as the required timescales commonly exceed practical computational limits. To overcome this, enhanced sampling techniques, such as replica exchange MD (REMD), have gained popularity because of their capability to accelerate free-energy barrier crossing and enrich configurational sampling. Over the past decade, numerous REMD variants have emerged, including multi-dimensional exchange schemes and hybrid approaches. The proliferation of these variants reflects the diversity of molecular systems (from small peptides to larger macromolecules) and the continued drive to improve sampling efficiency while rigorously preserving the correct target ensemble [1-4].

REMD runs multiple replicas of the system in parallel (e.g., different temperatures or Hamiltonians) and exchanges the conformations among them at fixed intervals. This exchange reduces correlation times and improves sampling efficiency by allowing the system to overcome kinetic barriers through transitions into neighboring states with lower barriers. Effective REMD requires moderate overlap in configurational space between neighboring replicas to facilitate efficient exchanges. Therefore, traditional REMD often demands a large number of closely spaced replicas to achieve optimal exchange rates, partially negating its computational advantage.

Here, we introduce Replica Exchange with Flexible Timing (REFT), a novel REMD variant that decouples exchange attempts from the fixed exchange time by permitting exchanges between adjacent replicas at variable, earlier time points relative to the scheduled exchange evaluation. This flexible timing elevates exchange rates and thereby reduces the computational cost for obtaining a given amount of sampling. While we conceived this novel approach for the purpose of calculating adsorption free energies for disordered adsorbants, we demonstrate the method's validity by obtaining accurate solvation free energies for small molecules and sampling the conformational ensembles of short peptides.

This work was supported by the Research Foundation Flanders (FWO) (project number G015022N). The supercomputing resources and services used in this work were provided by the VUB and the VSC (Flemish Supercomputer Center, project 2025_078), the latter being funded by the FWO and the Flemish Government.

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CAI - D1 - F01
Impact of fast mechanistic studies in industrial setting

Oriana Brea[1], Roel Hoefnagels[1], Mikko Muuronen[1]
[1]Janssen Research & Development, A Division of Janssen Pharmaceutica NV, a Johnson & Johnson company, Belgium

Quantum chemical reaction mechanistic studies may influence the discovery of chemically stable drug candidates and the optimization of synthetic processes. However, accurate quantum chemical studies are often deemed too costly for guiding experimental design. In this work, we demonstrate how first-principle mechanistic studies may contribute to molecular design during drug discovery and for optimizing synthetic reaction conditions within fast-paced industrial timelines when paired with selected experiments. Our study also underscores the accuracy required to guide experiments effectively and discusses the necessity of microsolvation in specific cases.

CAI - D1 - F02
Addressing process challenges through AI: Biobased amine production in flexizyme

Peter Baets[1]
[1]*Process Design Center, The Netherlands*

The world is facing a transition towards more sustainable circular feedstocks and processes, a strategic change that is promoted by the European Union. The EU-funded FLEXIZYME project, develops the production of bio-based fatty amines (FAs) from side stream materials, using innovative enzymatic conversion processes. FLEXIZYME is a 4-year project, with the aim of developing a flexible, cost-efficient biotechnological platform where innovative technologies concerning the catalyst and process design will be implemented. It considers all the development steps to obtain biobased FAs from fat rich and protein-rich feedstocks to fit real industrial needs.
The sustainability advantages that are expected from this approach rely on fundamental differences with traditional processes due to (a) the use of milder operating conditions (b) high selectivity of enzymes and (c) reduced energy needs of the biobased route. Together, these features contribute to a reduced environmental footprint and greater process efficiency.
Key challenges in this approach are, amongst others, related to product purification, downstream processing and overall process economics. In order to address these, PDC contributes to this project through conceptual process design, leveraging advanced digital tools such as Prosyn-AI[1] and state-of-the-art process simulators. Prosyn-AI is an extensive heuristic/numerical process synthesis AI-tool build by experts. It contains modules as depicted below that assist expert-users in process design choices (Prosyn-AI at PDC).
Prosyn-AI is used amongst others to support the techno-economic analysis, perform flow-sheeting, in house literature search and estimate physical properties of compounds. An example of the use of Prosyn-AI will be demonstrated at the conference.

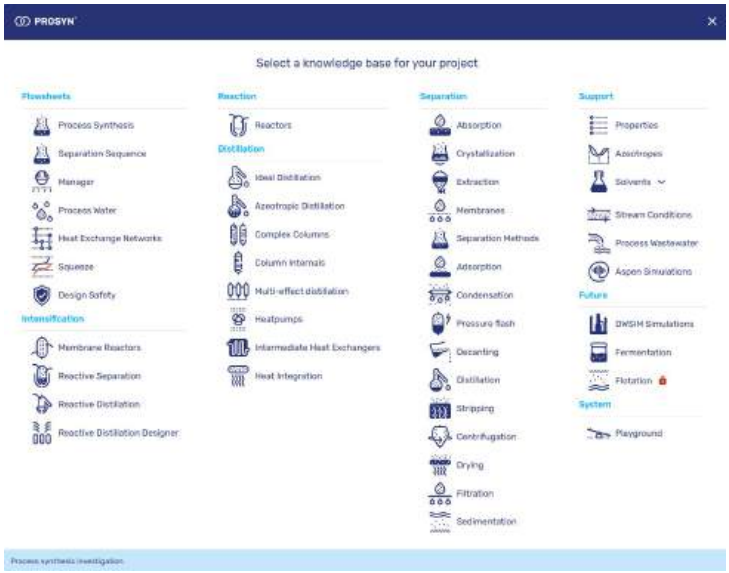

Fig. 1. Prosyn-AI modules

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or Circular Bio-based Europe Joint Undertaking. Neither the European Union nor the granting authority can be held responsible for them.

CAI - D1 - F03
In silico engineering of piezoelectric biomolecular assemblies

Geetu Kumari[1], Shubham Vishnoi[1], Sarah Guerin[1,2*]
[1]Dept. of Chemical Sciences, Bernal Institute, University of Limerick, Ireland; [2]SSPC, The Science Foundation Ireland Research Centre for Pharmaceuticals, University of Limerick, Ireland

The ability of certain materials to generate electric charge in response to mechanical stress is derived from their non-centrosymmetric crystal structures, which produces a wide array of applications in sensing, actuation, and energy harvesting[1]. Organic molecular crystals, present a promising platform for the next generation of piezoelectric materials[2]. Utilizing Density Functional Theory (DFT), we have developed CrystalDFT - a structured database of crystals accompanied by predicted electromechanical properties[3]. This dataset reveals a diverse range of piezoelectric responses, featuring a considerable number of materials exhibiting natural (unpoled) longitudinal piezoelectricity, which is essential for conventional piezoelectric applications. A focused study was also carried out on hydrated organic crystals[4], performing a high-throughput DFT screening and identifying thirty hydrates with longitudinal piezoelectric coefficients exceeding 10 pC/N. These results underscore the significance of hydrogen bonding in enhancing dipole alignment and facilitating polar crystal phases. These results led us to further investigate structure - property relationships, where we designed and synthesized a series of halogenated pyridin-3-ol derivatives (2-X-pyridin-3-ol; where X = Cl, Br, I). These crystals, stabilized by both hydrogen and halogen bonding[5], demonstrate high DFT-predicted shear piezoelectric responses of up to 99.19 pC/N. Experimentally-validated shear response of 54–74 pC/N in were accompanied by longitudinal responses ranging from 5 to 10 pC/N. Overall, these studies showcase the effectiveness of computational screening and molecular design in steering the discovery of high-performance organic piezoelectrics, bridging the gap between theoretical insights and practical applications in the development of sustainable electromechanical materials.

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CAI - D2 - O01
Training of machine-learned force fields for modeling metal–support interactions in catalysis

Martijn Hut[1], Alexander Bagger[2], Eelco T.C. Vogt[1], Bert M. Weckhuysen[1]
[1]Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, The Netherlands; [2]Catalysis Theory Center, Technical University of Denmark, Denmark

Metal–support interactions (MSIs) play a crucial role in heterogeneous catalysis, as they can significantly influence catalyst stability, activity, and selectivity. A comprehensive understanding of these effects requires not only advanced bulk and surface characterization techniques preferentially under reaction conditions, but also accurate computational modeling using density functional theory (DFT).[1] However, DFT calculations of supported metal nanoparticles are often limited by system size, leading to the use of idealized models that may fail to capture key MSI features.[2] Machine-learned force fields (MLFFs) provide a way to overcome this limitation by dramatically accelerating calculations and enabling simulations of larger systems. Frameworks, such as MACE[3], enable the construction of highly accurate MLFFs tailored to specific materials through the fine-tuning of foundational models.
Here, we present two strategies to cost-effectively fine-tune a MLFF for cobalt-based catalysts. More specifically, we have chosen Co/TiO_2 (Fig. 1) as model system, which is known to be active in the catalytic hydrogenation of CO and CO_2. The resulting MLFF achieves sufficient accuracy to investigate cobalt interactions with two TiO_2 polymorph surfaces (rutile and anatase) and enables the discovery of novel configurations for cobalt nanoparticles on TiO_2-anatase, wherein interfacial oxygen atoms actively bind to the cobalt nanoparticle, thereby altering the local chemical environment and potentially influencing reactivity (Fig. 2). This demonstrates the importance of the usage of MLFFs in MSI research. The rapid screening of structures allows the discovery of interface configurations that are computer cost prohibitive to conventional DFT methods.

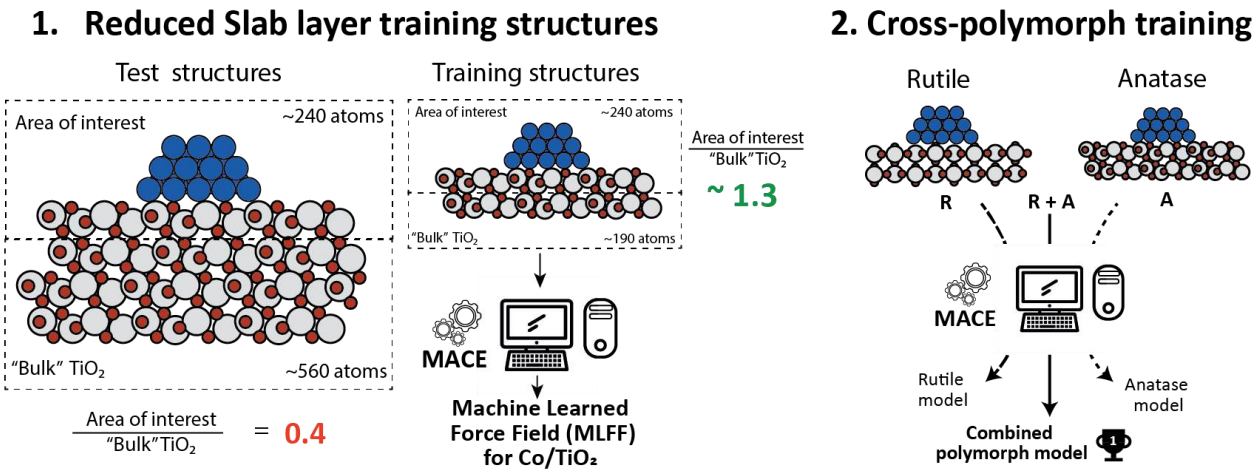

Fig. 1. Overview of two machine learned forcefield (MLFF) training strategies for supported Co nanoparticles on TiO_2: 1. Reduction number of support layers in training structures to increase information density of area of interest per training structure 2. Cross-polymorph training, to exploit MLFF transferability.

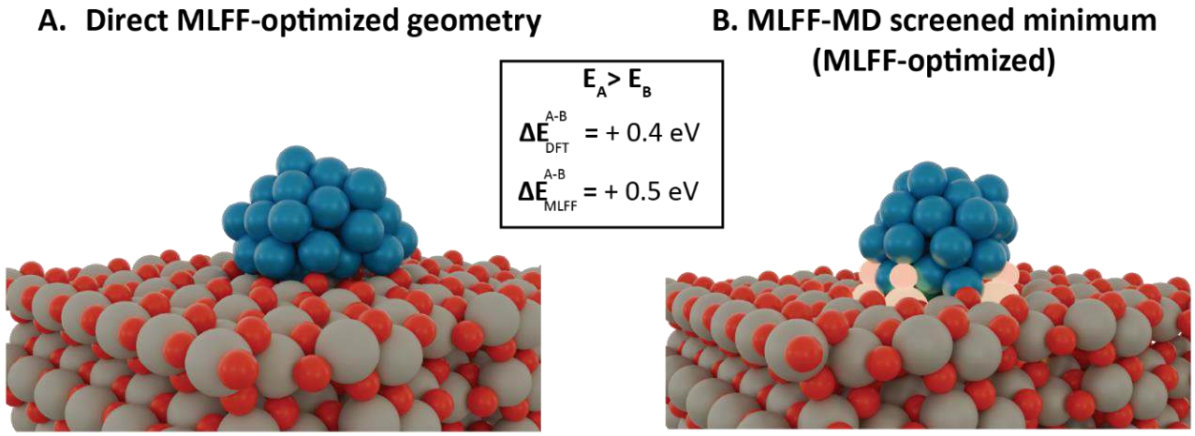

Fig. 2. Optimized geometries of a Co_{41} nanoparticle supported on TiO_2 - anatase obtained through optimization using the optimized machine learned force field (MLFF): (A) Geometry optimized from an idealized starting configuration and (B) Geometry optimized from an molecular dynamics (MD)-screened minimum, where the MD simulation was initiated from the same idealized starting configuration as in (A).

Bert Weckhuysen acknowledges Advanced Research Center Chemical Buildings Block Consortium (ARC CBBC) and NWO for financial support.

[1] Liu, J.; Chen, L.; Liu, X. *ACS Catal.* **2024**, *14*, 1987-2002.
[2] Sun, G.; Sautet, P. *Acc. Chem. Res.* **2021**, *54*, 3841-3849.
[3] Batatia, I.; Kovacs, D.; Simm, G.; Ortner, C.; Csányi, G. *Adv. Neur. Inf. Proc. Sys.* **2022**, arXiv:2206.07697.

CAI - D2 - O02

SimPoly: Simulation of polymers with machine learning force fields derived from first principles

Gregor N. C. Simm[1], Jean Hélie[1], Hannes Schulz[1], Yicheng Chen[1], Guillem Simeon[2], Anna Kuzina[1], Ernesto Martinez-Baez[2], Piero Gasparotto[2], Gabriele Tocci[2], Chi Chen[2], Yatao Li[1], Lixue Cheng[1], Zun Wang[1], Bichlien H. Nguyen[1], Jake A. Smith[1], Lixin Sun[1]

[1]Microsoft Research, AI for Science, UK; [2]Microsoft Quantum, USA

Polymers are a versatile class of materials with widespread industrial applications. Advanced computational tools could revolutionize their design, but their complex, multi-scale nature poses significant modeling challenges. Conventional force fields often lack the accuracy and transferability required to capture the intricate interactions governing polymer behavior. Conversely, quantum-chemical methods are computationally prohibitive for the large systems and long timescales required to simulate relevant polymer phenomena. In this work, we overcome these limitations with a machine learning force field (MLFF) approach. We demonstrate that macroscopic properties for a broad range of polymers can be predicted ab initio, without fitting to experimental data. Specifically, we develop a fast and scalable MLFF to accurately predict polymer densities, outperforming established classical force fields. Our MLFF also captures second-order phase transitions, enabling the prediction of glass transition temperatures. To accelerate progress in this domain, we introduce a benchmark of experimental bulk properties for 130 polymers and an accompanying quantum-chemical dataset. This work lays the foundation for a fully in silico design pipeline for next-generation polymeric materials.

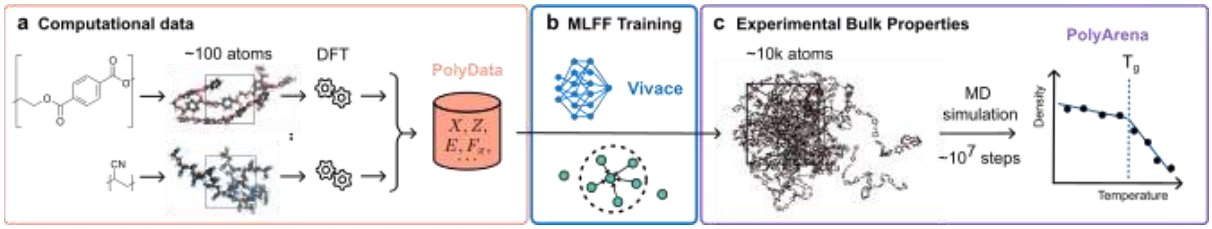

Fig. 1. Prediction of experimental bulk properties for a wide range of polymers through MD simulations with a MLFF trained solely on ab initio data.

[1]Simm, G. N. C.; Hélie, J.; Schulz, H.; Chen, Y.; Simeon, G.; Kuzina, A.; Martinez-Baez, E.; Gasparotto, P.; Tocci, G.; Chen, C.; Li, Y.; Cheng, L.; Wang, Z.; Nguyen, B. H.; Smith, J. A.; Sun, L. SimPoly. *Simulation of Polymers with Machine Learning Force Fields Derived from First Principles*. arXiv, **2025**. https://doi.org/10.48550/arXiv.2510.13696.

CAI - D2 - O03

AI-driven generative and rational design of peptide modulators targeting GUCY2C for Parkinson's disease

Elpiniki Paspali[1], Lars van der Heide[2], Ioana Ilie[1]

[1]University of Amsterdam, Van 't Hoff Institute for Molecular Sciences, The Netherlands; [2]University of Amsterdam, Swammerdam Institute for Life Sciences, The Netherlands

Parkinson's disease (PD) represents a major neurological disorder with limited disease-modifying therapies. Evidence suggests that guanylate cyclase C (GUCY2C) signaling may play a role in modulating neurodegenerative mechanisms, positioning GUCY2C as a promising therapeutic target[1]. Addressing the challenge of rationally designing peptide modulators with high affinity and specificity, we integrate state-of-the-art generative machine learning models with rational structure-guided design to create novel peptide candidates tailored to bind the GUCY2C receptor.

Our computational workflow begins with the generation of diverse peptide sequences and structures via generative models trained on sequence-structure data. These candidates are filtered in silico using predictive metrics for stability and binding potential. We then apply rational design heuristics informed by receptor binding energetics and structural compatibility to refine candidates[2]. Selected peptides are assessed through molecular dynamics simulations, docking and energy evaluation against the native peptides, prioritizing predicted affinity and favorable physicochemical properties.

We report a set of optimized peptide designs showing enhanced predicted binding with GUCY2C compared with baseline controls, highlighting the synergy between AI-assisted generative design and classical rational optimization. This work demonstrates a computational platform for rapid peptide discovery and underscores the potential of data-driven approaches to accelerate therapeutic design for neurodegenerative diseases.

[1]Douma, E. H.; Stoop, J.; Lingl, M. V. R.; Smidt, M. P.; van der Heide, L. P. *Cell Biosci.* **2024**, *14*, 132.

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CAI - D2 - O04

Computationally driven exploration of the structure and electronic properties of Cu_2GeSe_3 for use in high-performance thin film photovoltaic alloys

Philippa U. Cox[1], Alexander G. Squires[1], Peter P. Russell[1], Romain Claes[1], David O. Scanlon[1]
[1]School of Chemistry, University of Birmingham, UK

Ternary diamond-like copper chalcogenides are amongst the highest performing single-junction thin film photovoltaic materials. They exhibit lower toxicity and greater stability than CdTe and perovskite photovoltaics, while maintaining high performance at reduced film thicknesses relative to silicon. The highest performer $Cu(In,Ga)Se_2$ has reached a record power conversion efficiency of 23.6% at less than 2.0μm[1]. However, industry applications are limited due to the high-cost elements and the precise synthesis required to minimize performance-reducing defects. As a result, developing new thin film photovoltaic materials remains an important area of research.

Cu_2GeSe_3 has been explored as a thermoelectric for many years, it contains a larger proportion of cheap, non-toxic and abundant materials than CIGS, with good thermal and chemical stability. Previous work by the Scanlon Materials Theory Group has identified the silicon analogue Cu_2SiSe_3 as a promising defect tolerant photovoltaic material with a high theoretical power conversion efficiency of 30%[3]. The germanium system may offer promising properties as a bottom layer for tandem cells or alloy in photovoltaic thin films. However, little is known about the structure and properties of Cu_2GeSe_3. Once believed to be ordered, Cu_2GeSe_3 has now been shown to be more complex. It is essential to comprehensively characterise Cu_2GeSe_3 to ensure its suitability as a photovoltaic material.

This work explores the structure and properties of Cu_2GeSe_3. Our approach uses machine learning interatomic potentials to calculate the vibrational free energies of a range of structures for use in cluster expansions for Monte Carlo simulation-based disorder studies.

[1]Green, M.A et al. *Progress in photovoltaics: research and applications*. **2024**, *32*(7), pp.425-441.
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[3]Nicolson, A et al. *Journal of Materials Chemistry A*. **2023**, *11*(27), pp.14833-14839.

CAI - D2 - O05

Collisional cross-section prediction of peptides and small molecules: Covering all bases and bridging the gap

Robbe Devreese[1,2], Arthur Declercq[1,2], Alireza Nameni[1,2], Alexander Kensert[1,2], Ralf Gabriels[1,2], Lennart Martens[1,2,3,4], Robbin Bouwmeester[1,2]

[1]VIB Center for Medical Biotechnology, Belgium; [2]Dept. of Biomolecular Medicine, Ghent University, Belgium; [3]BioOrganic Mass Spectrometry Laboratory (LSMBO), University of Strasbourg, France; [4]Infrastructure Nationale de Protéomique, Strasbourg, France

Ion mobility–mass spectrometry (IM–MS) provides access to gas-phase molecular conformations, with the collision cross-section (CCS) serving as a key structure–property descriptor. Accurate CCS prediction remains challenging due to the sensitivity of IM to molecular flexibility, chemical functionalization, charge localization, and the presence of multiple gas-phase conformers and protomers.

Here, we present two deep learning approaches for CCS prediction that explicitly address these challenges across peptides and small molecules. IM2Deep models CCS as a function of molecular composition and modification, accurately predicting CCS values for peptides carrying arbitrary chemical modifications, including functional groups not observed during training (Figure 1)[1]. Furthermore, by training on a carefully curated dataset containing experimentally observed multiconformational peptide ions, IM2Deep improves prediction accuracy for both single and multiconformational peptides[2].

GraphXSection, on the other hand, is a graph neural network that learns structure-CCS relationships directly from molecular graphs. The model generalizes across diverse chemical classes and ion adducts, outperforming existing graph-based approaches (Figure 2). Incorporation of charge localization information enables accurate prediction of CCS for distinct protomers of the same molecule, highlighting the importance of intramolecular electrostatics in shaping gas-phase structure. Transfer learning further extends predictive performance to chemically challenging classes such as per- and polyfluoroalkyl substances (PFAS).

Finally, we evaluate GraphXSection on peptide CCS prediction, exploring a one-architecture-fits-all-approach for CCS prediction.

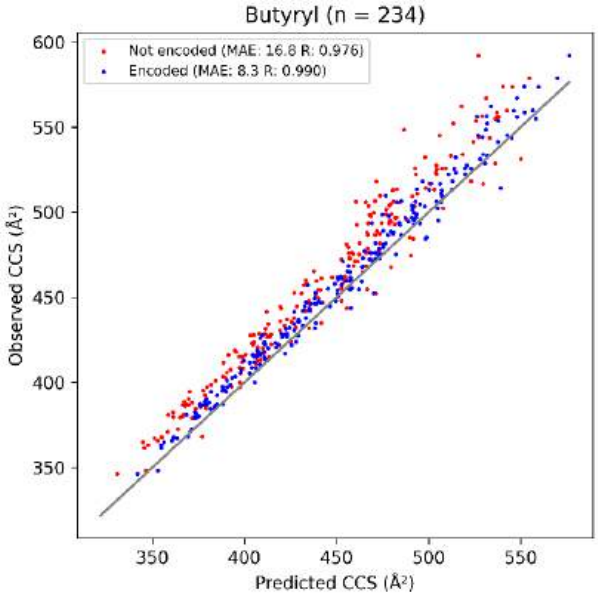

Fig. 1. Scatterplot illustrating the performance of the IM2Deep model not trained on butyrylated peptides ir predicting CCS for butyrylated peptides. The model was evaluated both with the modification encoded (blue) and ignored (red). Besides an improvement in mean absolute error, an increase in Pearson correlation coefficient is also seen. Variable n denotes the total number of butyrylated peptides.

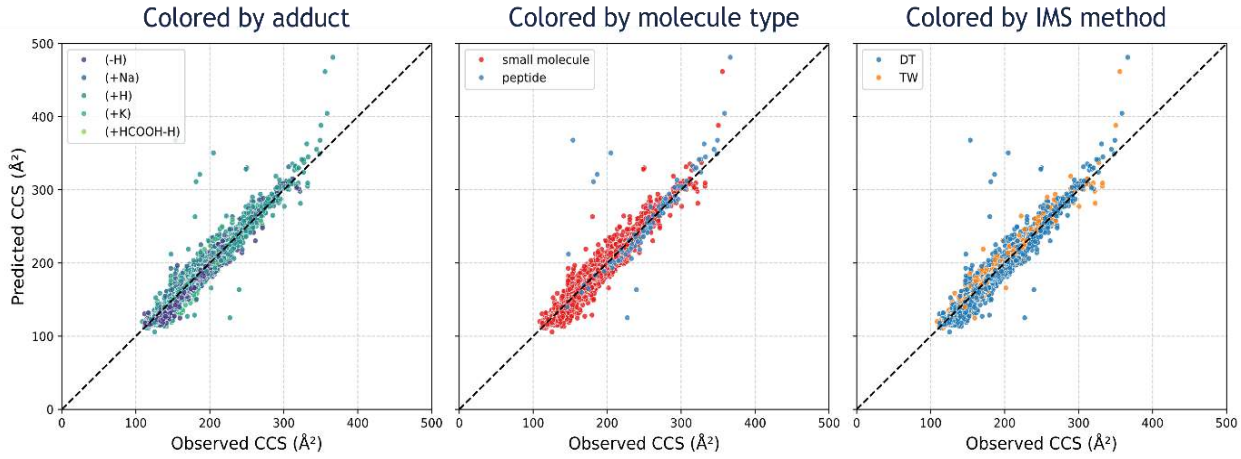

Fig. 2. Performance of GraphXSection on the CCSBase test dataset. As shown, GraphXSection shows excellent performance generalizing across ion adducts (left), molecule classes and even IMS methods (right).

[1]Declercq A. and Devreese R *et al. J. Proteome Res.* **2025**, *24*, 3, 1067–1076.
[2]Devreese R. *et al. Anal. Chem.* **2025**, *97*, 28, 15113–15121.

CAI - D2 - O06
Machine learning potentials at speeds comparable to reactive force fields

Loïc Dumortier[1], Kendrick Di Piro[1], Benoît Creton[2], Theo De Bruin[2], Jelle Vekeman[3], Toon Verstraelen[1]
[1]Center for Molecular Modeling (CMM), Ghent University, Belgium; [2]IFP Nouvelles, France; [3]Modelling and Simulation in Chemistry (MOSAIC), University of Antwerp, Belgium

Machine learning potentials (MLPs) provide quantum-chemical accuracy with significantly greater computational efficiency than first-principles methods. However, their cost is still high compared to empirical force fields, which limits applicability for simulations over extended time and length scales. While empirical force fields excel in computational speed, they do so at the expense of accuracy. This work explores strategies to optimize the computational efficiency of MLPs while maintaining physical accuracy and model stability. The goal is to enable simulations at scales comparable to or exceeding reactive force fields, but with superior accuracy. Furthermore, the MLPs should enable the description of multiple spontaneous reactive events in a realistic chemical environment. We propose an active learning framework that minimizes human intervention while generating a compact, yet diverse and representative training set. Using kernel density estimation on node energies, our method effectively identifies and targets out-of-distribution structures, eliminating the need for computationally intensive ensemble approaches. We benchmark the resulting MLP against ReaxFF[1] and the general-purpose MACE-MP-0 model[2], evaluating performance in terms of accuracy, efficiency, and ability to capture chemical reactivity. Our approach is applied to a hydrated silicate ionic liquid (HSIL)—a chemically complex system relevant to zeolite synthesis. The dedicated model supports stable integration at a 1.2 fs timestep, achieving up to a 10x speedup over MACE-MP-0 and a 5x improvement over ReaxFF, while also accommodating systems 10 times larger in GPU memory than MACE-MP-0. In comparison, ReaxFF and MACE-MP-0 both underestimate the density of HSIL, whereas our model accurately reproduces densities at dilute compositions and slightly overestimates them in low-water-content systems. Long-timescale simulations further confirm that the MLP captures chemical reactivity in the liquid phase. Overall, this work demonstrates that carefully tailored MLPs can outperform empirical force fields in both accuracy and efficiency, offering a scalable and cost-effective solution for reactive molecular dynamics.

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[2]Batatia, I et al., *J. Chem. Phys* **2025**, *163*, 148110.

CAI - D2 - O7

Quantum chemistry is all you need: Data-free inverse molecular design with PROTEUS

Francesco Calcagno[1,2], Luca Serfilippi[1], Giorgio Franceschelli[1], Marco Garavelli[1], Mirco Musolesi[1,3], Ivan Rivalta[1,2]

[1]University of Bologna, Italy; [2]Center for Chemical Catalysis, Italy; [3]University College London, UK

Molecular inverse design is considered as a *Holy Grail* in Chemistry thanks to its potentially disruptive applications in the development of new functional molecules and materials.[1] In recent years, machine learning (ML) has become a key tool for fast prediction of molecular properties as well as generation of new compounds.[1] However, ML models usually require large datasets for being trained, limiting their broad applications and potentially introducing biases in generation. For these reasons, data-free generative models are gaining more attention as they do not need any initial training set to work.[2,3]

In this contribution, we present PROTEUS, a data-free ML method for *de novo* molecular design.[2] The tool implements a deep reinforcement learning algorithm that generates molecules as ASCII strings. The quality of generated candidates is evaluated through an online computational prediction of the target property using quantum chemistry software packages. Thanks to the direct quantum mechanical feedback, PROTEUS rapidly learns to improve the generation of candidates while converging on (sub)optimal solutions.[2]

We successfully tested the capabilities of PROTEUS in designing styrene derivatives featuring target isomerization energies computed at density functional theory (DFT) level. Numerical simulations showed that PROTEUS efficiently explores the chemical space, finding optimal candidates without requiring any pre-training and outperforming a baseline.[2] Thanks to its general and data-free implementation, PROTEUS paves the way for transferable quantum chemistry driven molecular design.

[1]Freeze, J. G.; Kelly, H. R.; Batista, V. S. *Chem. Rev*. **2019**, *119*, 6595–6612.
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[3]Calcagno, F.; A. Cabral, D. G.; Rivalta, I.; Batista, V. S. *arXiv* **2025**, 2508.15896.

CAI - D2 - O08

Packed by the surface: Relating surface structure and solvation properties at solid/water interfaces

Mohammed Bin Jassar[1*], Simone Pezzotti[1*]
[1]*Laboratoire CPCV, Dépt. de Chimie, École Normale Supérieure, PSL University, Sorbonne University, France*

Our progress in interfacial chemistry has traditionally relied on understanding how surfaces interact directly with reactive species. However, a growing number of studies[1,2,3] highlight an equally important, indirect role of surfaces: reshaping the local solvation environment. This effect is challenging to rationalize, arising from a subtle interplay between the water network and surface properties, which limits our ability to predict interfacial reactivity[1]. Here, using machine learning, we show that it can be quantitatively predicted with a single descriptor -- the packing of interfacial water molecules. Leveraging the new descriptor, we construct a minimal phenomenological model to predict solvation free energies at solid/liquid interfaces, validated across diverse surfaces. The model provides intuitive insights for engineering solvation effects in interfacial chemistry.

This work is funded by the European Research Council (ERC, ELECTROPHOBIC, Grant Agreement No. 101077129). This work was performed using HPC resources from GENCI, allocation No. A0170802309.

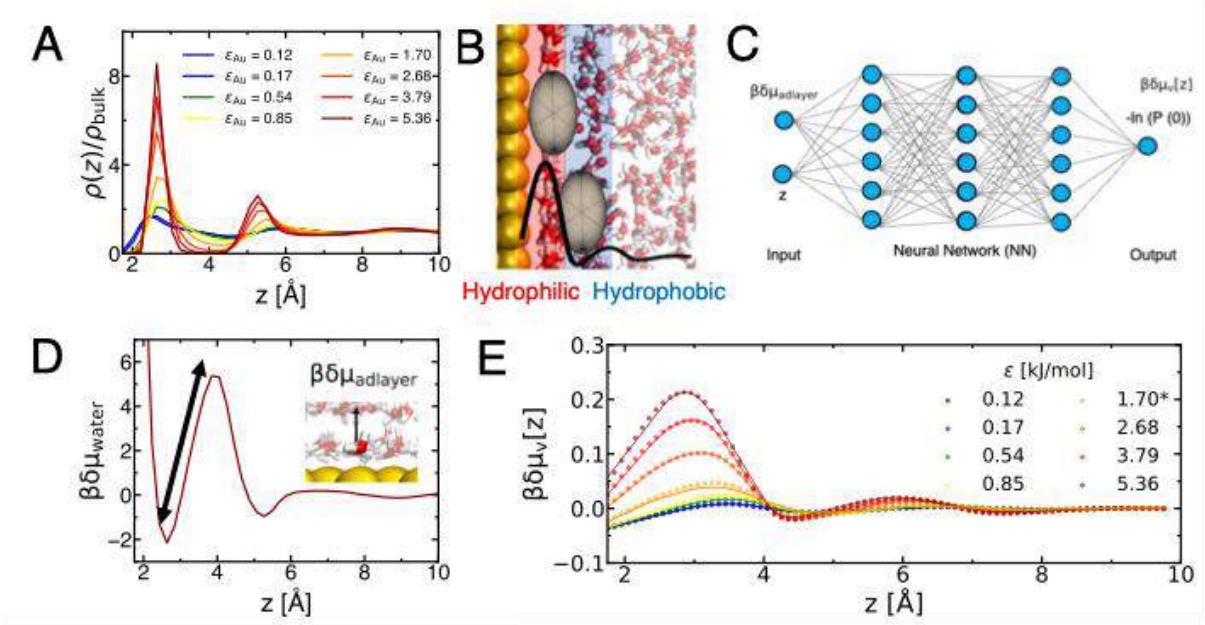

Fig. 1. shows several key aspects of the study. Panel A presents density profiles across various interfaces with different surface–water interaction strengths. Panel B illustrates a schematic of the hydrophobic solvation free energy across the gold/water interface. Panel C depicts the architecture of a neural network that takes two inputs and produces a single output. Panel D shows the free energy cost of removing water from the adlayer, which defines the degree of packing. Finally, panel E demonstrates that the neural network successfully reproduces molecular dynamics (MD) data.

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[2]Murke, S; et al. J. Am. *Chem. Soc*. **2024**, *146*, *18*, 12423–12430.
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CAI - D2 - O09

Chemoinformatics profiling of Annona muricata-derived compounds targeting COX-2 in breast cancer

Krishna Kuben Govender[1,2], Vitalis Mbayo[1], Vincent Adeiza Obakachi[1], Penny Poomani Govender[1]
[1]University of Johannesburg, South Africa; [2]National Institute for Theoretical and Computational Sciences, South Africa

Breast cancer remains one of the leading causes of cancer-related mortality globally, with a disproportionate impact in low- and middle-income countries, with cyclooxygenase-2 (COX-2) overexpression promoting tumour progression, angiogenesis, and therapy resistance. This study explored the chemical diversity of Annona muricata (soursop) to identify potent COX-2 inhibitors using an integrated in silico workflow. A library of 52,242 natural compounds was screened through high-throughput virtual screening and Glide extra-precision (XP) docking against COX-2 (PDB ID: 3LN1). From 104 preliminary hits, 27 leads were prioritised via Prime MM/GBSA ($\Delta G_{bind} \leq -70$ kcal/mol), and DFT optimisation (M06-2X/def2SVP) highlighted five top candidates: Tellimoside, Hamamelitannin, Catechin-4-ol 3-O-α- L-rhamnopyranoside, Avicularin, and Myricetin-3-O-arabinofuranoside. Tellimoside exhibited the highest affinity (Glide score: −13.58 kcal/mol; post-DFT ΔG_{bind}: −79.64 kcal/mol), forming sixteen stabilising interactions within the COX-2 active site. Molecular dynamics simulations (350 ns, AMBER20) confirmed the complex's stability (RMSD: 2.27–2.83 Å; RMSF < 1 Å), structural compactness (RoG < 24.00 Å), and reduced solvent exposure. Post-simulation MM/GBSA analysis reaffirmed strong binding (ΔG_{bind}: −74.21 kcal/mol), driven by van der Waals and electrostatic forces. Subsequently, frontier molecular orbital (FMO) analysis further demonstrated high electronic reactivity (ΔE: 5.50 eV; softness: 0.36 eV^{-1}), indicating favourable adaptability within the active site. These results suggest that A. muricata-derived polyphenols, particularly Tellimoside, are computationally predicted scaffolds for selective COX-2 inhibition and may serve as adjuvant therapeutics that may guide future experimental validations for breast cancer management.

CAI - D2 - O10
Uncertainty-aware prediction of ^{195}Pt chemical shifts from limited data

Alexander Messler[1], Hilke Bahmann[1]
[1]*University of Wuppertal, Germany*

Platinum (Pt) complexes are highly relevant for medicinal chemistry and homogeneous catalysis.
In the development of novel Pt-based chemotherapeutic agents and catalysts, characterization of the compounds using nuclear magnetic resonance (NMR) spectroscopy of the ^{195}Pt nucleus is standard.
However, measuring ^{195}Pt-NMR signals can be tedious due to the large chemical shift range and limited resolution. To facilitate experimental measurements by narrowing down the shift range, reliable predictions of the chemical shift are needed. Especially for lighter nuclei such as ^{1}H and ^{13}C, machine learning (ML) methods predict chemical shifts accurately, while analogous models for heavier nuclei are scarce. In this work[1], we propose Gaussian Process Regression models for the prediction of ^{195}Pt chemical shifts. The underlying dataset comprises 292 structures[2,3] and three different descriptors were used to encode structural and chemical features of the molecules. Based on the prediction uncertainties derived from the posterior variance of the models, a reasonably narrow shift range can be estimated for a given Pt complex. The most robust model was obtained by applying the Smooth Overlap of Atomic Positions descriptor, whose hyperparameters were tuned using Bayesian optimization, enabling efficient exploration of the hyperparameter space and substantially improving predictive performance. This model yields a mean absolute error of 114 ppm on the holdout test set, which is significantly more accurate than relativistic DFT calculations.

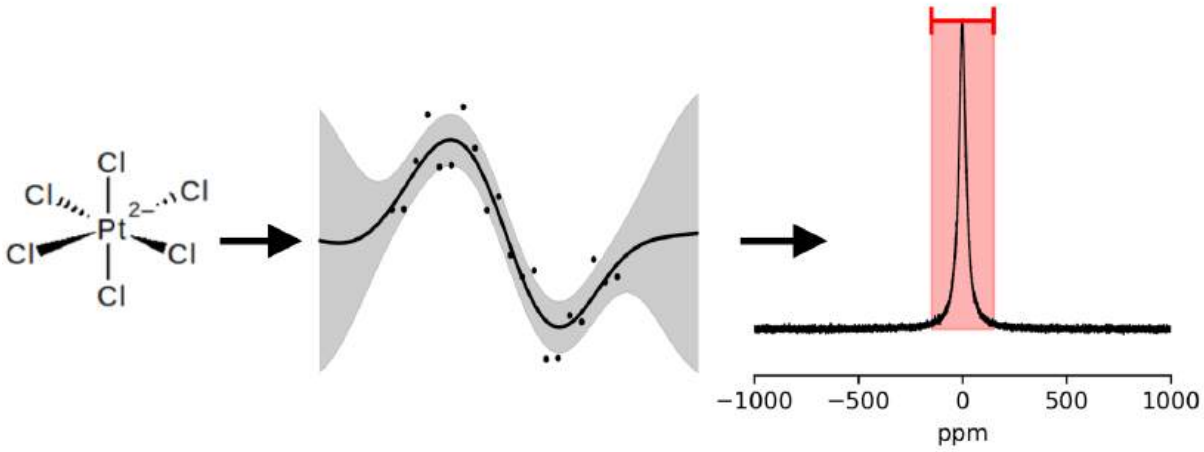

Fig. 1. Using a Gaussian process regressor to predict the chemical shift of a given Pt complex. The model provides the prediction and exact Bayesian uncertainty measures as given by the predictive variance of the regressor.

[1]Messler, A. & Bahmann, H. *J. Chem. Inf. Model.* **2026**, *accepted manuscript.*
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[3]Ondar, E. et al. *ChemPhysChem* **2023**, *24*, e202200940.

CAI - D2 - O11
Machine learning force fields for accelerated design and discovery of electrocathodic materials

Muhammad Umer[1], Matthias Vandichel[1]
[1]*University of Limerick, Republic of Ireland*

The development of efficient and durable catalysts for electrochemical reactions remains a key challenge in sustainable energy technologies. Commercial catalysts rely predominantly on noble metals such as Pt, Ru, Ir, and Pd, however, their high cost, limited availability, and sluggish reaction kinetics hinder large-scale application.[1] A promising strategy is to develop low-cost, stable, and efficient electrocatalysts capable of stabilizing reaction intermediates and lowering kinetic barriers.[2] Two-dimensional materials, particularly non-precious-metal-based single-atom/dual-atoms catalysts supported on MXenes, MBenes, graphene, and hexagonal boron nitride (*h*-BN), offer tunable electronic structures and high atomic utilisation.[3] Nevertheless, establishing structure-activity relationships in these candidate structures remains challenging.
Elucidating atomic-scale relationships requires systematic exploration of broad chemical and configurational spaces. While density functional theory (DFT) provides accurate atomistic insights, it becomes computationally expensive when applied at large scales, limiting comprehensive exploration and screening. To overcome this limitation, machine learning (ML) assisted atomistic modelling offers an effective approach for accelerating materials discovery while retaining first-principles accuracy.[4-6] To this end, we employed an automated DFT-based machine learning framework, in which energies, forces, and stresses were calculated using the Vienna *ab initio* Simulation Package with the PBE exchange-correlation functional. On-the-fly machine learning force fields are generated using sparse Gaussian process regression, as implemented in the AutoForce package. Continuous integration of newly generated DFT data enables the ML potential to adapt dynamically as updated coordinates are sampled. This integrated framework significantly reduces computational cost and screening time while maintaining predictive reliability. Preliminary results for *h*-BN-based model systems indicate improved structural stability and favourable HER activity following structural optimization, demonstrating that this approach provides a systematic and efficient route for exploring complex electrochemical reactions and guiding for the development of next-generation electrocatalysts for sustainable energy applications.

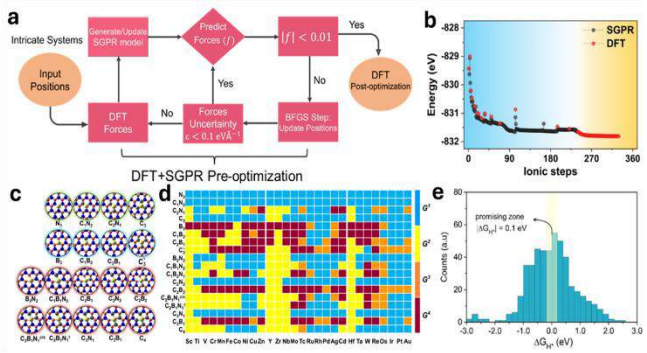

Figure 1. (a) DFT+SGPR workflow, **(b)** energy convergence landscape showing SGPR efficiently approximates DFT, **(c)** various h-BN SAC structures, **(d)** stability heatmap, and **(e)** ΔG_{H^*} distribution highlighting the promising catalytic zone for HER.

Acknowledgments: M.V. acknowledges funding from Research Ireland under the Frontiers for the Future Programme (MEM-E-TECH, 23/FFP-A/12221) and from the Horizon Europe research and innovation programme (SUN2CN, Grant Agreement No. 101223193). M.U. and M.V. acknowledge the Irish Centre for High-End Computing (ICHEC) for providing computational facilities and support.

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CAI - D2 - O12
FFLUX: Machine learnt potentials based on quantum topological atoms

Paul L.A. Popelier[1], O. Aten[1], P. Bandyopadhyay[1], M. Brown[1], J. Chung[1], L. Cabrera[1], G. Hawe[1], B. Isamura[1], Y. Manchev[1], M. Nosratjoo[1], A. Pák[1], M. Vincent[1]
[1]Dept. of Chemistry, University of Manchester, UK

We pioneered [1] the use of Gaussian Process Regression in atomic potentials. Contrary to other research groups we started with the machine learning (ML) of electrostatics. We covered all 20 amino acids [2] because FFLUX [3] targets protein simulation. Electrostatics manifests itself at long-range and, in order to reach the exact limit, one must work with multipole moments. Next followed accurate ML predictions of the atomic energies using quantum topological atoms [4], such that a single partitioning method provides all atomic properties. This uniformity guarantee accuracy for the right reasons and hence future-proof work. Sustained in-house software delivered the training program FEREBUS [5] supported by pipeline ICHOR [6] and the MD program DL_FFLUX. ML methods such as grey-wolf optimisation are used for the first time [7] with superior performance. The parallellisation [8] of DL_FFLUX enables the simulation of condensed matter, whether molecular crystals [9] or liquid water [10], all with polarisable electrostatics. We also reached a proof-of-concept replacing Lennard-Jones potentials for both repulsion [11] and dispersion [12]. FFLUX simulations show unprecedented robustness [13] with competitive CPU-times.

Acknowledgement: PP is grateful for an ERC Advanced Grant.

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CAI - D2 - O13

Data-centric AI in computational chemistry: Integrating curated literature with spectrometry and microscopy to accelerate trustworthy discovery

Sergey Varnavskiy[1]
[1]Elsevier GmbH, Germany

AI in chemistry is only as powerful as the data it learns from. We present a data-centric, human-in-the-loop framework in which curated literature and reaction data from chemistry-related curated database (Reaxys) provide the backbone for reproducible, explainable pipelines in computational chemistry and CADD. Normalized reactions, structures, properties, and bioactivities with transparent provenance and interoperable schemas enable:

(i) literature-anchored, interpretable retrosynthesis routes traceable to precedents [1];
(ii) mechanism-informed impurity prediction across multi-step syntheses (including genotoxic risks); and
(iii) forward synthesis and digital experimentation with uncertainty quantification, model cards, and actionable explanations.

We integrate three complementary AI modules with the curated database.

1) Learning-to-rank models that digitize chemists' intuition of molecular complexity from expert-labeled data, improving dataset characterization, guiding route selection, and revealing topology–complexity trends across drug discovery and total synthesis [2].

2) An isotope-distribution–centric ML search engine that mines tera-scale high-resolution mass spectrometry archives to practice "experimentation in the past," rigorously interrogating existing spectra to uncover overlooked transformations (e.g., vinyl–NHC coupling in Mizoroki–Heck) and to validate literature precedents without new experiments [3].

3) FAIR archiving and ML-assisted analysis of electron microscopy, addressing the >90% rate of lost unpublished images and unlocking hidden structural information to strengthen mechanism and impurity forecasts [4].

Case studies demonstrate that curated database-anchored pipelines enhance generalization, reduce bias via provenance-rich curation [1], and close the loop from prediction to experiment through automated HRMS mining and microscopy reuse [3, 4]. This integrated approach—combining curated literature (Reaxys), spectrometry, and microscopy with interpretable ML—delivers safer, faster, and greener chemical innovation while setting a practical path to trustworthy AI in chemistry.

Acknowledgements: The author thanks colleagues for discussions on data-centric AI and access to curated literature resources.

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CAI - D2 - O14

Data-driven process intensification of methyl acetate production via surrogate-based Bayesian optimization

Trung N Trinh[1], Trung Thanh Nguyen[2], Roman Tschentscher[1], Nikolaos Tsakoumis[1]
[1]SINTEF Industry, Process Technology, Trondheim, Norway; [2]Faculty of Information Technology- Da Nang University of Science and Technology, Vietnam

Direct carbonylation of dimethyl ether (DME) with carbon monoxide is an attractive route for methyl acetate (MeAce) production, offering integration within C1-based value chains. However, strong nonlinear interactions between reaction conditions, recycle structure, and compression energy demand limit the effectiveness of conventional simulation-based optimization.

This work presents a data-driven process intensification framework combining steady-state process simulation, machine-learning surrogate modeling, and Bayesian optimization (BO). Approximately 3000 steady-state operating points were generated using a design-of-experiments (DOE) strategy based on a literature-derived kinetic flowsheet of the DME carbonylation process implemented in the CoCo process simulator. Five operating variables—reactor temperature, reactor length, reactor pressure, CO feed rate, and purge splitter ratio—were varied to explore the design space (see Fig.1).

Residual neural network models delivered the most accurate and robust surrogate model, providing reliable predictions within and beyond the training domain. Embedded within a Bayesian optimization framework, the surrogate replaces the computationally expensive process simulator and enables efficient exploration of continuous, high-dimensional design spaces. The model predicts C-yield, defined as the fraction of carbon converted to MeAce relative to the total carbon fed via DME and CO, together with the specific compressor energy consumption per unit mass of MeAce produced (SCEC).

Multi-objective Bayesian optimization reveals a narrow, well-defined optimal operating window in which MeAce carbon yield is maximized while specific energy consumption is minimized, before entering the Pareto region where trade-offs become unavoidable. The maximum carbon yield identified by BO exceeds that obtained from the DOE dataset by approximately 9%. As the system moves into the Pareto region, carbon conversion increases from 85% to 94%, while SCEC rises from 0.15 to 0.26 MJ kg^{-1} MeAce (see Fig.2). Validation using rigorous CoCo process simulations confirms the reliability of the framework, with deviations below 4% for C-yield and 17% for SCEC at the optimal zone.

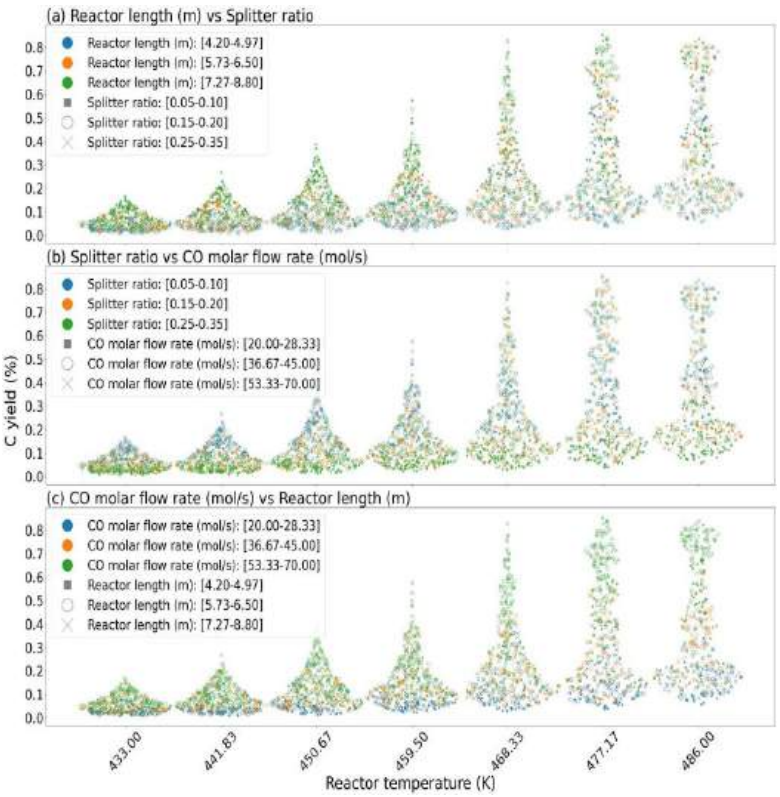

Fig. 1. *Effects of reactor temperature, reactor length, splitter ratio, and CO molar flow rate on MeAce production (*Pressure and SCEC are not shown in this figure).

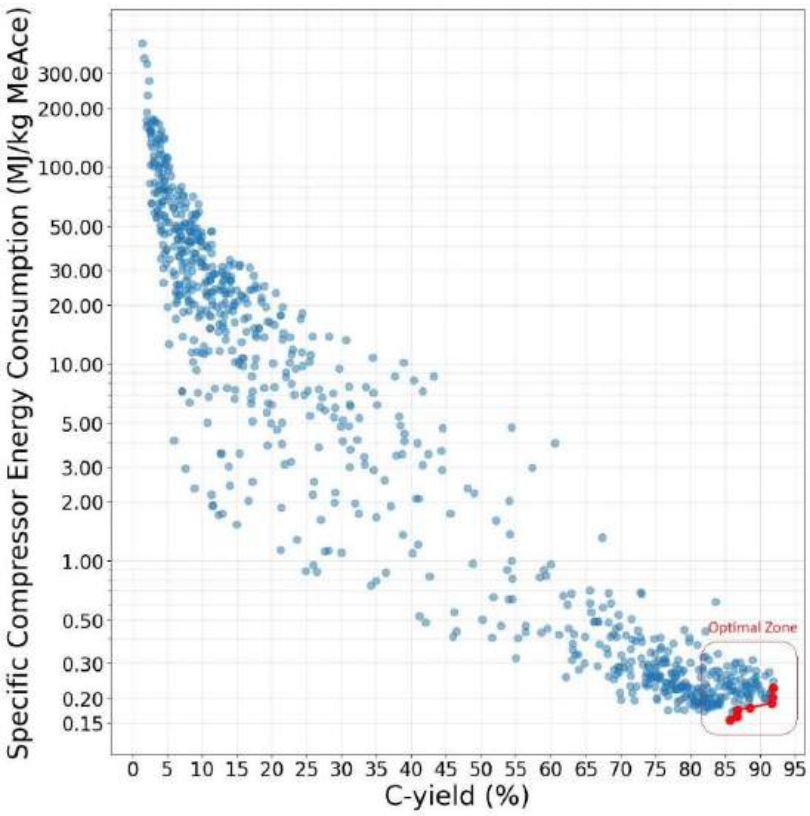

Fig. 2. Bayesian optimization process and Pareto-front solutions (in red points) for the trade-off between carbon yield and specific compressor energy consumption.

CAI - D2 - O15
Exploring the mechanism of protochlorophyllide to chlorophyllide conversion

Elham Sattarinezhad[1,2], Stefano Raniolo[3], Marco Garavelli[1,2], Vittorio Limongelli[3], Ivan Rivalta[1,2]
[1]*Dept. of Industrial Chemistry "Toso Montanari", University of Bologna, Italy;* [2]*Center for Chemical Catalysis – C3, University of Bologna, Italy;* [3]*Faculty of Biomedical Sciences, Università della Svizzera italiana (USI), Institute of Computational Science, Switzerland*

Light-driven chlorophyll biosynthesis involves the reduction of protochlorophyllide (Pchlide) to chlorophyllide by the enzyme protochlorophyllide oxidoreductase (POR) in the presence of the NADPH cofactor. This reaction is essential for plant development and provides a distinctive system for investigating enzymatic catalysis occurring under low-temperature conditions and on ultrafast timescales.[1] Understanding the underlying photochemical mechanism critically depends on accurate structural knowledge of the POR–NADPH–Pchlide ternary complex.[1]

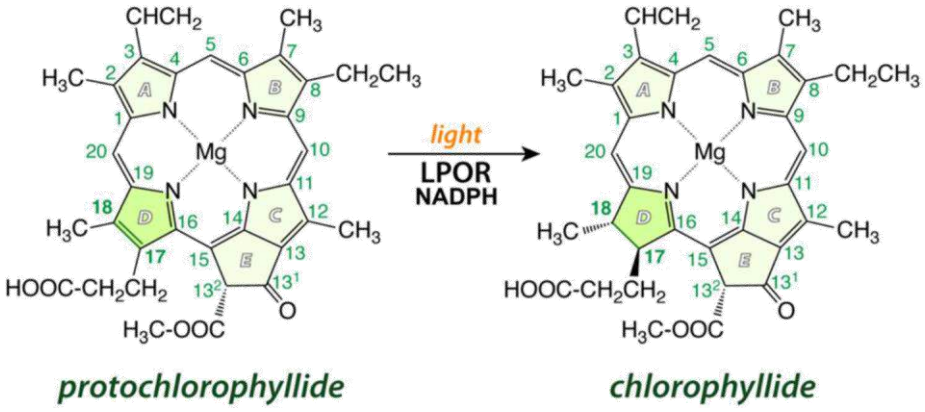

Fig. 1. A scheme of the reaction catalyzed by LPOR[2]

While crystal structures are available for cyanobacterial LPOR variants, these structures lack the bound Pchlide substrate,[3] limiting mechanistic interpretation. Conversely, recent cryo-EM models provide complete ternary complexes but at relatively low resolution,[4] leaving the substrate orientation within the active site insufficiently resolved. This structural ambiguity remains a major obstacle to mechanistic characterization. In this work, starting from experimentally derived structural models, we employed funnel well-tempered metadynamics simulations to explore and characterize plausible binding orientations of Pchlide within the LPOR active site. Enhanced sampling enables systematic mapping of the substrate free-energy landscape and identification of energetically favorable binding modes compatible with catalytic geometry. The resulting structural ensembles provide refined starting configurations suitable for subsequent QM/MM investigations aimed at elucidating the reaction pathway. This integrative computational strategy contributes toward resolving the structural determinants governing LPOR photoreactivity and advances molecular-level understanding of light-driven enzymatic catalysis.

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CAI - D2 - O16
Lone-pair shielded radicals: Beyond the captodative substitution pattern

Steven E. Beutick[1,2], Maarten J. H. van Dorp[1], Trevor A. Hamlin[1], J. Martijn van der Schuur[2], Daniela Rodrigues Silva[1], F. Matthias Bickelhaupt[1]
[1]Vrije Universiteit Amsterdam, The Netherlands; [2]Nouryon, The Netherlands

The influence of substituents on the C–C bond strengths is commonly rationalized in terms of radical stabilization by electron-donating groups. Here, we revisit the C–C bond using quantitative molecular-orbital (MO) theory based on relativistic DFT. The C–C bond in 1,2-disubstituted ethanes $RH_2C–CH_2R$ becomes progressively weaker as the electron-donating ability of the substituent R increases along the series R = F, H, CH_3, OH, and NH_2.
Our analyses show that this trend originates from the presence of a lone-pair shielded radical (LPSR) on $RH_2C^{\bullet}$ radicals, in which a lone-pair-like lobe of an occupied orbital surrounds the radical electron and hampers the formation of the C–C electron-pair bond via Pauli repulsion. The LPSR on $RH_2C^{\bullet}$ arises from the bonding combination of a lone-pair on the substituent R and the $2p_z$-type SOMO on the carbon center (Figure 1a). As the lone pair on the substituent is at high energy, *e.g.*, for R = NH_2, it is more electron donating, causing the RSLP to obtain a larger amplitude on the carbon center. As the lone pair drops to a lower orbital energy, the RSLP has a smaller amplitude on carbon, leading to less destabilization across the C–C bond and thus a stronger bond.
Contrary to the widely accepted explanation, we show that, except for R = F, substitution destabilizes the $RH_2C^{\bullet}$ radical. The substituents still weaken the C–C bond because they destabilize the parent molecule more than the corresponding radicals. Overall, this work demonstrates the generality of the lone-pair shielding effect, beyond captodative radicals, and can be used as a handle for tuning the bond strengths.[2]

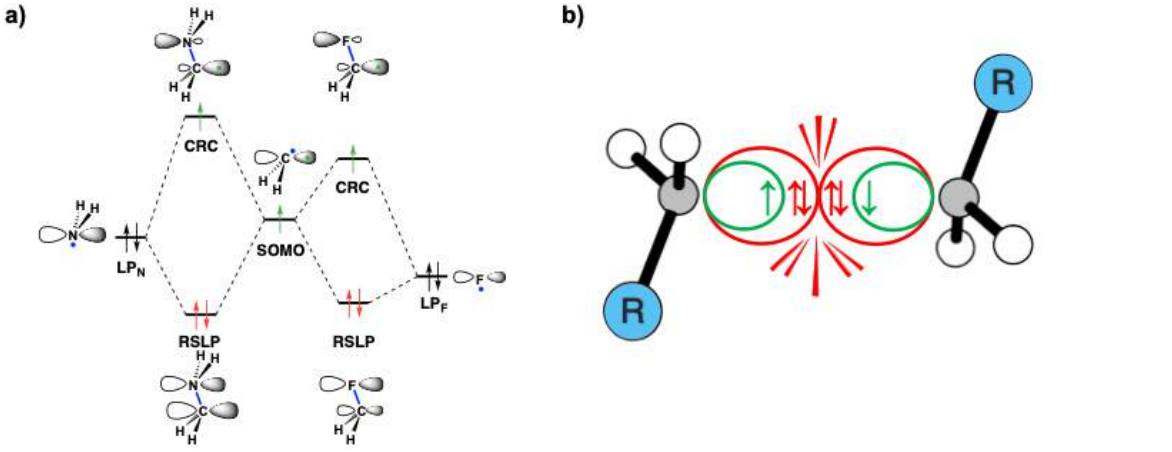

Fig. 1. a) Schematic orbital interaction diagram between $H_2C^{\cdot\cdot}$ and $R^{\bullet}$ (for R = NH_2 and F) for the formation of the radical shielding lone-pair (RSLP, red) and the carbon radical center (CRC, green) that is involved in the pair bond. The orbital interaction associated with the C–R electron pair bond (blue) is not shown. b) A graphic representation of the lone-pair shielded radical.

We thank Nouryon and the Netherlands Organization for Scientific Research (NWO) for financial support.

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CAI - D2 - O17

Novel computational strategies for the study of chemical selectivity: Combining high accuracy and chemical insight

Giovanni Bistoni[1]

[1]Dept. of Chemistry, Biology and Biotechnology, University of Perugia, Italy

In this contribution, we present a comprehensive computational framework that integrates high-level quantum chemical methods, advanced sampling techniques, and data-driven models to study chemical selectivity in complex molecular systems. Specifically, we combine coupled cluster-based electronic structure methods for accurate energy evaluations,[1] enhanced conformational sampling protocols capable of identifying relevant low-energy structures of both solute and solvent within a hybrid implicit/explicit solvation scheme,[2] and quantitative energy decomposition and electronic structure analysis tools.[3] To further improve the accuracy and transferability of the protocol, we incorporate machine learning models trained to correct systematic errors and enhance predictive performance. As an illustrative application, we employ this integrated approach to investigate the reaction mechanism and stereocontrolling factors of a previously reported asymmetric transformation.[4]

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CAI - D2 - O18
ORCA meets python – The ORCA python interface OPI

Christoph Plett[1], Tim Tetenberg[1], Hagen Neugebauer[1], Markus Bursch[1], Christoph Riplinger[1]
[1]FACCTs GmbH, Germany

Quantum chemistry has become an integral part of chemical research and facilitates the development of transformative technologies in fields such as materials science, pharmaceuticals, and catalysis. Alongside methodological advances, increasingly efficient and accessible software packages have made quantum chemistry a routine tool for addressing a wide range of chemical challenges. ORCA, one of the most widely used quantum chemistry software packages, is particularly valued for its efficiency, robustness, and versatility. Beyond enabling diverse chemical applications, such capabilities also support the rapidly growing field of machine-learning-based computational chemistry by facilitating the generation of large, high-quality datasets, such as Open Molecules 2025 (Omol25),[1] for training robust and transferable models.
In this context, the seamless integration of quantum chemistry software into modern, Python-based workflows has become increasingly important. To address this need, we have developed an open-source ORCA Python Interface (OPI),[2] which provides direct, programmatic access to ORCA's extensive methodological toolkit from within Python. OPI offers an ORCA-native abstraction of methods, basis sets, and calculation types, enabling fine-grained control over ORCA-specific functionality through a modular, object-oriented API.
In this talk, we present an overview of OPI, including its design philosophy, technical architecture, and core features. Application examples demonstrate how OPI enables the automated setup, execution, and analysis of quantum-chemical workflows, including high-throughput calculations across large molecular libraries, systematic benchmark studies involving multiple theoretical methods and basis sets, and detailed analyses of chemical phenomena based on quantum-chemical data.
By promoting script-based, shareable workflows, OPI enhances reproducibility and transparency in computational chemistry. In doing so, it standardizes ORCA-based workflows and lowers the barrier to scalable quantum-chemical calculations, empowering expert users and newcomers to perform computational studies and data generation more efficiently, systematically, and reproducibly.

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CAI - D2 - O19

Computational screening of triphenylamine-based star-shaped molecules: Insights into electronic and optical properties for organic photovoltaic

Pinar Seyitdanlioglu[1], Hilal Kalkan[2], Baris Temelli[1]
[1]Hacettepe University, Turkiye; [2]Gazi University, Turkiye

Star-shaped π-conjugated small-molecule donors have attracted increasing interest in organic photovoltaic (OPV) research due to their broad light absorption ranges, isotropic charge transport, and favorable film-forming properties. However, systematic studies elucidating the role of terminal acceptor engineering within a fixed star-shaped π-congugated core architecture remain limited. In this work, a rational computational design and screening study of triphenylamine (TPA)-based star-shaped donor molecules is presented with the aim of revealing structure–property relationships relevant to OPV performance[1,2].

A molecular library consisting of six star-shaped donor molecules sharing the same three-armed TPA core and π-bridging units, but differing in their terminal heteroaromatic acceptor groups, was designed. Ground-state geometries were optimized using density functional theory (DFT), and frontier molecular orbital energy levels (HOMO/LUMO), band gaps, and charge-transport-related reorganization energies were determined. Time-dependent density functional theory (TD-DFT) calculations were performed to investigate optical and excited-state properties.

The results demonstrate that terminal acceptor units play a decisive role in governing the electronic structure and photophysical behavior of star-shaped donors. This study demonstrates that terminal acceptor engineering constitutes a key molecular parameter in the rational design of star-shaped OPV donors and clearly highlights the effectiveness of computational screening in guiding material selection prior to synthesis. The presented findings provide a robust theoretical framework for the development and experimental validation of next-generation star-shaped donor materials.

Keywords: Organic photovoltaics, star-shaped molecules, triphenylamine, DFT, TD-DFT, computational screening

Acknowledgements: The computations carried out in this study were performed using the TRUBA resources of the TÜBİTAK ULAKBİM High Performance Computing Center. This work was supported by the Gazi University Scientific Research Projects Coordination Unit (BAP Project No: 10789).

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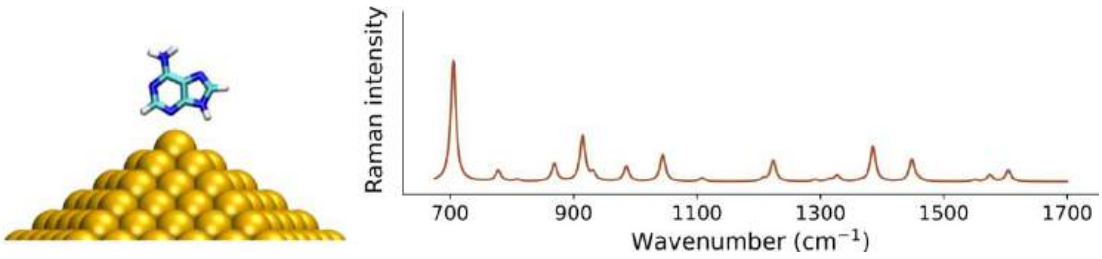
CAI - D2 - O20
Driving chemistry through plasmonic photoinduced phenomena: An atomistic perspective

Tommaso Giovannini[1]
[1]*University of Rome, Tor Vergata, Italy*

The optical response of plasmonic nanostructures can be tuned by varying their shape, size, and chemical composition [1]. When a molecular system interacts with the surface of plasmonic materials, a range of distinctive phenomena can emerge, from surface-enhanced spectroscopies to photocatalysis [2]. Capturing the optical properties of plasmonic substrates with high accuracy is therefore essential to understand the underlying physical mechanisms driving the chemistry at the interface. Here, we present a classical yet atomistically detailed approach for predicting the plasmonic behavior of nanostructures with arbitrary geometries. The method is general enough to handle a wide variety of plasmonic materials [3,4]. We demonstrate that our classical plasmonics model accurately replicates both ab initio reference data [3] and experimental observations [3,4], and is scalable to large nanoplasmonic systems (exceeding 1 million atoms). By incorporating the atomistic representation, our method can describe systems characterized by quantum effects, such as subnanometer junctions [3,5] and picocavities [6].
We also address the current challenges in modeling plasmonic photoinduced phenomena at molecule-nanostructure interfaces. In particular, we present a novel multiscale approach that couples the atomistic, yet classical description of the plasmonic nanostructure with a quantum mechanical treatment of the adsorbed molecular system. The resulting method enables the simulation of surface-enhanced spectroscopies, with particular emphasis on Surface-enhanced Raman Scattering (SERS), and photoinduced processes governed by local field enhancement [7-8].



This work has received funding from the ERC under the European Union's Horizon Europe research and innovation programme (grant no. 101219149, project CHOPIN). Views and opinions expressed are however those of the author only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

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CAI - D2 - F01

Structure-based discovery of NLRP3 inflammasome inhibitors: An integrated computational approach combining virtual screening, molecular dynamics, and binding free energy calculations

Cumhur Gokhan Ekmekci[1]
[1]*Independent Researcher, Istanbul, Turkey*

The NLRP3 inflammasome is a validated therapeutic target for inflammatory disorders including atherosclerosis, gout, type 2 diabetes, and neurodegenerative diseases. Despite pharmaceutical interest, selective small-molecule inhibitors targeting the NACHT domain remain limited. We present an integrated computational strategy to identify novel NLRP3 inhibitors through structure-based approaches.

A multi-tier virtual screening was conducted against the NLRP3 NACHT domain (PDB: 7ALV). Initial compound selection from ChEMBL database using Tanimoto-based clustering yielded 635 diverse candidates. Molecular docking employed AutoDock Vina with exhaustiveness of 16 and 32 for tier-1 and tier-2 screening. The top-ranked compound underwent 10 ns molecular dynamics simulation using GROMACS 2023. Binding free energies were calculated via MM-GBSA (GB-OBC2 model, 0.15 M ionic strength) with per-residue decomposition. PubChem similarity searching (Tanimoto ≥ 0.7) expanded the chemical space, followed by QED scoring and Lipinski evaluation.

Tier-1 screening identified 68 compounds with scores below -10.0 kcal/mol. CHEMBL5290148 showed the best binding energy (-12.49 kcal/mol). Molecular dynamics confirmed stable protein-ligand interactions with ligand RMSD of 1.8 ± 0.3 Å and consistent hydrogen bonding throughout the trajectory. MM-GBSA revealed strong binding affinity (ΔG = -52.47 ± 2.99 kcal/mol), dominated by van der Waals contributions (39.4%) indicating deep hydrophobic pocket occupancy. Per residue decomposition identified eleven critical residues (ΔG < -1.0 kcal/mol), with LEU242 (-2.91 kcal/mol), ILE59 (-2.31 kcal/mol), and GLY58 (-1.99 kcal/mol) contributing most within the Walker A motif region. PubChem expansion yielded 283 analogues; eight demonstrated scores ≤ -11.0 kcal/mol. The most promising candidate (CID 54583713) exhibited favorable properties (MW: 383.4 Da, QED: 0.658, zero Lipinski violations) while maintaining the 1,2,4-oxadiazole pharmacophore.

This investigation establishes a framework for NLRP3 inhibitor discovery combining rapid virtual screening with thermodynamic validation. The identified binding determinants provide insights for optimization. Compounds bearing oxadiazole-piperidine scaffolds with fluorinated substituents represent starting points for medicinal chemistry programs targeting NLRP3-mediated inflammatory pathologies.

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CAI - D2 - F02

Structure-based identification of novel USP7 inhibitors targeting the p53-MDM2 axis: A computational approach for anticancer drug discovery

Cumhur Gokhan Ekmekci[1]
[1]*Independent Researcher, Turkey*

Ubiquitin-specific protease 7 (USP7) regulates the p53-MDM2 tumor suppressor pathway by stabilizing MDM2, which promotes p53 degradation. Inhibiting USP7 destabilizes MDM2 and restores p53-mediated apoptosis, offering a therapeutic strategy for wild-type p53-retaining cancers. Despite compounds like FT671 and XL188 reaching clinical evaluation, developing selective USP7 inhibitors with good drug-like properties remains difficult.

We conducted structure-based virtual screening against the USP7 catalytic domain. The protein structure was obtained from AlphaFold2 (UniProt: Q93009, pLDDT: 91.0) and the catalytic triad (Cys223, His464, Asp481) was defined as the binding site. A focused library of 50 compounds based on known USP7 inhibitor scaffolds (quinoline, indole, piperidine) was assembled following Lipinski criteria. Docking was performed using AutoDock Vina (exhaustiveness: 16). Top candidates were prepared for molecular dynamics using GROMACS with AMBER99SB-ILDN/GAFF2 force fields over 10 ns trajectories.

Screening yielded a 30% hit rate (15/50 compounds) at ≤-5.5 kcal/mol threshold. The best hit (ligand_41) showed -6.19 kcal/mol binding energy, comparable to reported USP7 inhibitors. Quinoline scaffolds dominated the results, with four compounds in the top five positions; hydroxyquinoline derivatives performed particularly well. Active compounds shared molecular weights of 219-280 Da and LogP values of 3.6-5.0, fitting lead-like space suitable for optimization. Fluoroindole-phenol derivatives represented an alternative chemotype with three hits below -5.8 kcal/mol. Molecular dynamics confirmed stable binding poses for the five prioritized candidates.

Our results identify quinoline-based compounds as starting points for USP7 inhibitor development. The structural resemblance between our hits and clinical candidates supports the screening approach. Given USP7's role in p53-MDM2 regulation, these compounds warrant further optimization through binding free energy calculations and biochemical validation toward preclinical development.

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CAI - D2 - F03

Mimicking the effect of displacement parameter and crystallographic resolution on the topology of electron density distributions: Application to non-covalent interactions

Laurence Leherte[1], Johan Wouters[1]

[1]Laboratoire CBS, Dept. of Chemistry, Namur Institute of Structured Matter (NISM), Namur Research Institute for Life Sciences (NARILIS), Namur Medicine & Drug Innovation Center (NAMEDIC), University of Namur, Belgium

The analysis of the topology of the electron density distribution (EDD) in molecular/crystalline systems, particularly through bond critical points (BCP), has become a widely used approach to describe non-covalent interactions (NCI).[1] Most of the studies reported in literature focus on highly detailed EDDs. In the present work, the influence of two crystallography factors, isotropic displacement parameter and crystallographic resolution, is investigated through convolution products applied to EDDs. A Gaussian[2] and a resolution filter are applied to mimic the effect of each factor, respectively. Studying filtered EDDs and their BCP property profiles may be seen as additional sources of information to classify BCP in terms of NCI types. The BCP properties of filtered promolecular and QM (DFT B3LYP 6-311++G**) EDDs are determined for a hydrated ligand-protein system (3UNK.pdb) and are interpreted in terms of NCIs. Gaussian and resolution filterings lead to different patterns of BCPs. As examples, while the halogen bond (XB) and salt bridge remain detected in highly smoothed EDDs regardless of the filter, the effect of water molecules is more pronounced in the resolution filtered results than in the Gaussian ones. Within the Gaussian-based filtering frame, the hydrogen bonds (HB) differ from the XB and van der Waals BCPs through the shape of the Laplacian (L) profiles (Figure). Apparent transitions of BCPs from NCI to covalent interaction (CI) type are also observed, e.g. through the sign of L. Using the resolution filtering mode, HB BCPs can be characterized by multiple NCI-to-CI changes, while other types of BCPs show only one transition at specific filtering degrees (Figure).

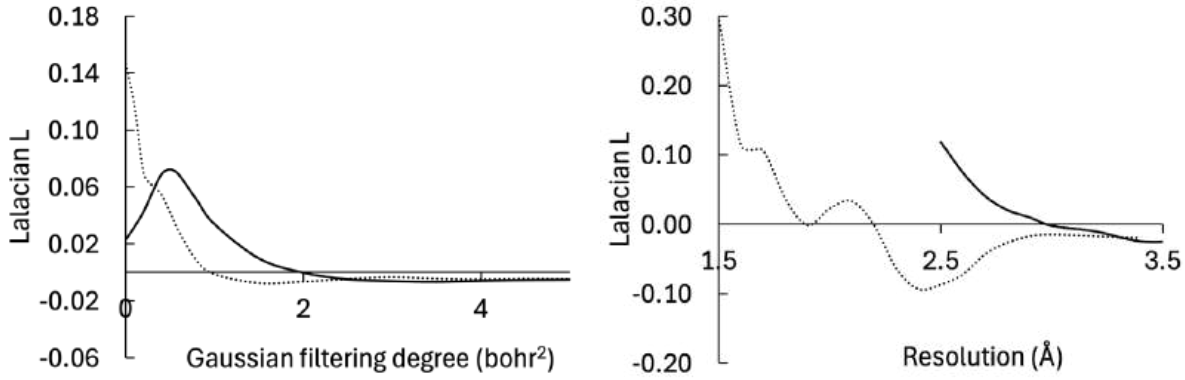

Fig. Laplacian profiles for the BCPs corresponding to a HB (dotted line) and a XB (plain line) protein-ligand interaction obtained from the Gaussian (left) and the resolution (right) filtering of QM EDDs.

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CAI - D2 - F04
How subsurface carbon affects hydrogen interactions at transition metal electrodes

Raju Lipin[1], Matthias Vandichel[1]
[1]*School of Chemical Sciences and Chemical Engineering, Bernal Institute, University of Limerick, Republic of Ireland*

Subsurface species can form or be explicitly engineered under reaction conditions and persist, quietly steering catalytic behavior, an effect increasingly recognized over the past decades.[1-2] The growing importance of subsurface carbon (C_{sub}) now extends to electrocatalysis, where a recent study shows that C_{sub} suppresses hydrogen absorption in palladium, thereby promoting selective alkyne semihydrogenation.[3-4] Motivated by this "hydrogen concentration knob," we examine how C_{sub} modulates hydrogen adsorption, and absorption on transition-metal electrodes. In this work, we use *ab initio* thermodynamics to construct phase and surface Pourbaix diagrams, which confirm C_{sub} tunes hydrogen adsorption and absorption across pH, potential, temperature, and pressure, shifting thresholds between surface binding and subsurface uptake. This framework identifies stability regimes in which C_{sub} enhances hydrogen availability relevant to the hydrogen evolution reaction or suppresses over-hydrogenation in selective hydrogenation reactions. More broadly, we show that subsurface species can be explicitly engineered to control hydrogen binding and diffusion, providing operando-testable, "carbiding-aware" design rules for transition-metal electrodes.

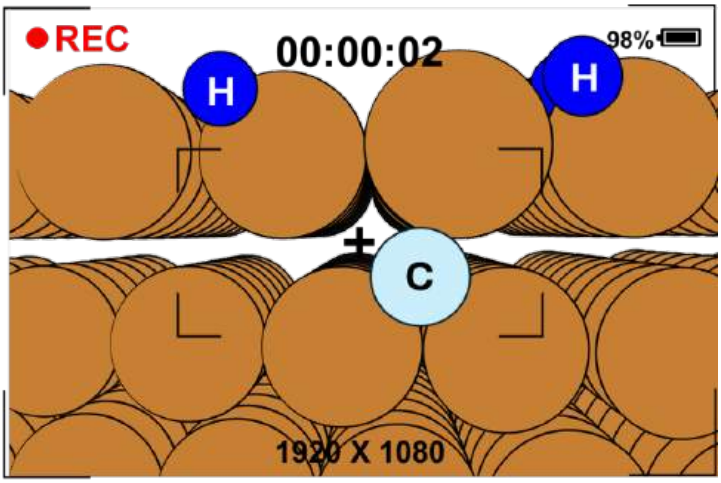

Fig. 1. Cartoon model showing a subsurface carbon atom in the sublayers of a metal electrocatalyst.

Acknowledgements. This work was funded by Research Ireland under the Frontiers for the Future Programme (MEM-E-TECH, 23/FFP-A/12221) and the Government of Ireland Postgraduate Fellowship (GOIPG/2025/1233). Computational resources were provided by the Irish Centre for High-End Computing (ICHEC).

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CAI - D2 - F05
Bridging chemical property explainability between chemistry and machine learning

Eugen Hruška[1], Fang Liu[2]
[1]Dept. of Biophysics and Physical Chemistry, Faculty of Pharmacy, Charles University, Czech Republic; [2]Dept. of Chemistry, Emory University, USA

Explaining chemical properties and their machine-learning models can improve our ability to understand chemistry. Here, we want to bridge two different chemical explanation approaches. On the one side, the atomwise and bondwise approach allows to assign to each atom or bond an attribution factor, but this factor does not always have a direct chemically valid interpretation. Another approach, the matched molecular pair analysis, maintains chemical validity, but the selection of pairs is not always unique. By constructing a set of chemical operations, we create explanations that are both atomwise/bondwise and chemically valid. We demonstrate this approach by analyzing the explainability of the HOMO-LUMO energy gap for a large set of molecules.[1]

[1]Hruska, E; Zhao, L.; Liu, F. *Ground truth explanation dataset for chemical property prediction on molecular graphs ChemRxiv.* **2022**, Preprint.

CAI - D2 - F06
FNDMC as a tool for quantifying static and dynamic electron correlation in complex systems

Katarína Šulková[1], Martin Šulka[1]
[1]Advanced Technologies Research Institute, Faculty of Materials Science and Technology in Trnava, Slovak University of Technology, Slovakia

The distinction between dynamic and non-dynamic (static) electron correlation is intuitively appealing and has long been recognized in quantum chemistry. Nevertheless, establishing a clear separation between these two components remains challenging, since both single-reference and multi-reference electronic structure methods capture aspects of each type of correlation to varying degrees. Recently, we have developed a method [1–3] that enables an unambiguous partitioning of the exact electron correlation energy into dynamic and non-dynamic contributions. This approach is based on the fixed-node diffusion Monte Carlo (FNDMC) method employing nodal surfaces derived from a restricted Hartree–Fock (RHF) Slater determinant. FNDMC with fixed RHF nodes recovers all dynamic correlation exactly, while the remaining portion of the correlation energy, denoted as E_{nd}, arises solely from the discrepancy between the imposed RHF nodal surface and the exact nodal structure. The proposed framework makes it possible to i) quantify the importance of static correlation in complex systems as will be demonstrated on energy decompositions of multiple systems, including small metal clusters and bond breaking of diatomic molecules, and, at the same time, to ii) assess the effectiveness of various electronic structure methods (e.g. CASSCF, CCSD(T), DFT) in recovering dynamic and non-dynamic correlation energy.

Acknowledgment: Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00435

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CAI - D2 - F07
Accurate property data for small molecules from theory

Dirk Andrae[1]
[1]*Freie Universität Berlin, Germany*

Property data for isolated small molecules in their electronic ground state, like molecular structure or fundamental frequencies, are highly important in many branches of science, e. g. astrochemistry, atmospheric chemistry, heterogeneous catalysis, matrix isolation vibrational spectroscopy under cryogenic conditions, to name just a few. But the "power of data" is misled if the data is of inferior quality. As is well known, calculated property data compare very well with experimental data (see, e. g., refs. 1, 2 and references therein), if (i) the system under study – the molecule in a given electronic state – is composed of only few and light atoms (say, $Z < 10$) and if (ii) the calculated property data derive from a sufficiently high level of quantum chemical theory (typically from an explicitly correlated method like CCSD(T)-F12). This contribution shows that property data for many small molecules containing heavier atoms (up to, say, $Z = 80$ [Hg]) can be accurately calculated with a valence-only treatment.

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CAI - D2 - F08

Control of quantum entanglement and electronic coherence in attosecond molecular photoionization

Adrián J. Suñer-Rubio[1,2*#], Lisa-M. Koll[3#], Tobias Witting[3], Roger Bello[4], Alicia Palacios[2,5], Fernando Martín[2,6], Marc J. J. Vrakking[3]

[1]UR Molecular Systems, Department of Chemistry, University of Liège, Belgium (current address); [2]Depto de Química, Universidad Autónoma de Madrid, Spain; [3]Max-Born Institute, Germany; [4]Depto de Química Física Aplicada, Universidad Autónoma de Madrid, Spain; [5]Institute of Advanced Research in Chemical Sciences, Universidad Autónoma de Madrid, Spain; [6]Instituto Madrileño de Estudios Avanzados IMDEA-Nanociencia, Spain

The advent of the first attosecond pulses[1,2] enables the study of ultrashort time-scale properties by coherently populating several continuum states due to the broad bandwidth of the pulses. However, very commonly, the ionization of these systems into an electron and its remaining ion leads to the production of an entangled electron-ion pair. This ion-photoelectron entanglement compromises the ability of attosecond pump-probe experiments to explore coherent ultrafast electron dynamics within ions or photoelectrons. Hence, the effect of entanglement in ultrafast photoionization processes has been explored recently in atomic[3-5] and molecular[6-8] systems.

Following the trend paved by previous works, here, a novel attosecond pump-probe scheme has been experimentally and theoretically tested in the photoionization of the hydrogen molecule. The scheme involves combining a phase-locked pair of XUV isolated attosecond laser pulses and a few-cycle near-infrared laser pulse. Within this scheme, the modulation of electronic coherence in the dissociating H2+ ion is achieved through the control of quantum entanglement between the photoelectron ejected into the continuum and the remaining molecular ion. As shown in Figure 1, this control is achieved by varying both the delay between the two XUV attosecond pulses and the delay between them and the few-cycle near-infrared pulse, highlighting the importance of properly considering quantum entanglement in optimally observing electronic coherences in attosecond experiments[9].

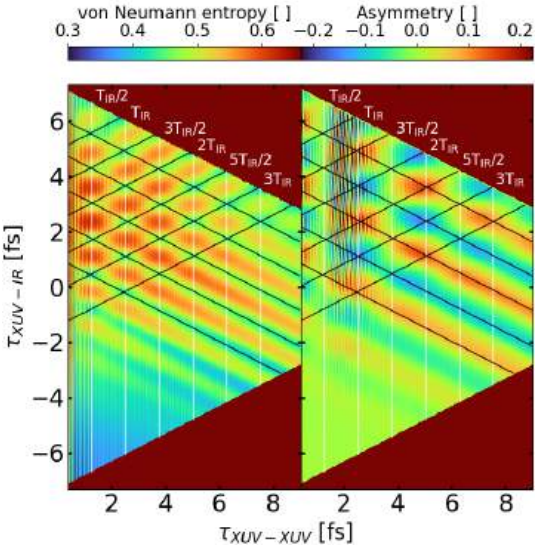

Fig. 1. Entanglement (left panel) and electronic coherence (right panel) as a function of both pulse delays. The vertical white lines cut the XUV-XUV delays written in white. The black diagonal lines have slopes of 1/2 and -1/2 and pass through the minima of the von Neumann entropy as well as through the maxima and minima of the asymmetry.

* E-mail: ajsuner@uliege.be. Adrián J. Suñer-Rubio is presently a 2026 IPD-STEMA post-doc in the group of Prof. Francoise Remacle at ULiège. # These authors contributed equally to this work.

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CAI - D3 - O01
Resolving spin contamination in spin-flip methods: The extended spin-flip CC2 method

Simen Camps[1], Daniel Escudero[1], Thomas-C. Jagau[1]
[1]KU Leuven, Belgium

Spin-flip (SF) methods[1,2] provide a great black-box alternative to multi-reference methods for the description of strongly correlated molecules. Starting from a high-spin single reference, the multi-configurational low-spin target states can be obtained by spin-flipping excitations. SF methods have been successfully applied to describe bond-breaking, diradicals, conical intersections and transition metal complexes.[2] However, the description of excited states is less straightforward because they are spin contaminated due to the incompleteness of the excitation space.[3] We developed a method within equation-of-motion coupled-cluster theory that closely resembles the SF extended configuration interaction singles (SF-XCIS) method[4] to reduce this incompleteness and obtain more accurate excitation energies for molecules with a multi-configurational ground state. This extended SF method yields different solutions for singlet and triplet excited states in contrast to the regular SF methods where higher lying excited states are a spin-contaminated mixture of both. Combined with second order approximate coupled-cluster theory (CC2),[5,6] we compare its performance with respect to full CI for small molecules such as methylene and to multi-reference CCSD for, for example, the different conformers of benzyne. Furthermore, we demonstrate the application range by computing excitation energies for larger molecules such as hexacene.

S.C. gratefully acknowledges the Research Foundation Flanders (FWO) for the received PhD fellowship (Grant No. 1152325N).

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CAI - D3 - O02

Machine learning and multireference configuration interaction for high-level nonadiabatic dynamics simulation of hexatriene

Hans Lischka[1], Richard A. Messely[2], Pavlo O. Dral[3,4,5], Mario Barbatti[6,7], Luan G. F. dos Santos[1], Mikołaj Martyka[8], Adélia J. A. Aquino[9], Julio C. V. Chagas[10,11], Francisco B. C. Machado[10,11]

[1]Dept. of Chemistry and Biochemistry, Texas Tech University, USA; [2]National Center for Computational Sciences, Oak Ridge Leadership Computing Facility, Oak Ridge National Laboratory, USA; [3]State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, and Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Xiamen University, China; [4]Institute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University Torún, Poland; [5]Aitomistic, Shenzhen, China; [6]Aix Marseille University, France; [7]Institut Universitaire de France, Paris, France; [8]University of Warsaw, Faculty of Chemistry, Poland; [9]Dept. of Mechanical Engineering, Texas Tech University, Lubbock, TX, USA; [10]Dept. of Chemistry, Aeronautics Institute of Technology, São José dos Campos, Brazil; [11]Advanced Scientific Computing and Modeling Laboratory, Aeronautics Institute of Technology, São José dos Campos, Brazil

Recently [1], we have shown how multireference configuration interaction (MR-CISD) available in the COLUMBUS program can be successfully applied to calculating the vertical excitation spectra from all-trans hexatriene to all-trans dodecahexaene and to perform geometry optimizations of the S_1 and S_2 states for hexatriene up to decapentaene, as well as to calculate the minimum on the crossing seam (MXS) between S_0 and S_1 for hexatriene.

Based on this experience, machine learning (ML) techniques have been used to enable MRCI-based photodynamics simulations, using all-trans hexatriene as the first benchmark. In the first step, the AIQM1 neural network-corrected method of MLatom [2] was used to perform surface-hopping (SH) dynamics using Newton-X [3], providing structural space for subsequent sampling of hexatriene photo-dynamics. Then, the total structural data set containing ~930,000 structures was reduced to a representative set of ~1000 structures using active learning. In the next step, MRCI calculations, including energies and energy gradients, were performed for the lowest three singlet states of each structure in the 1000-structure sample. Active learning has been used to reconstruct the entire energy surfaces using MRCI. Surface-hopping dynamics has been performed using an MRCI-trained neural network, leading, for the first time, to a photodynamics simulation of hexatriene at such a high computational level.

Alternatively, active learning and fine-tuning available in MLatom is being used to directly conduct SH dynamics calculations up to the size-extensivity corrected MR-CISD+P level.

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CAI - D2 - O03

Convex hartree-fock and density functional theory for stable simulations at conical intersections

Federico Rossi[1], Tommaso Giovannini[2], Henrik Koch[1]
[1]Norwegian University of Science and Technology, Norway; [2]University of Rome Tor Vergata, Italy

Conical intersections play a central role in photochemistry, energy relaxation, and radiationless transitions, yet they remain a major challenge for widely used electronic structure methods. Standard Hartree-Fock (HF) and Density Functional Theory (DFT) rely on a single-reference description with an asymmetric treatment of ground and excited states through their time-dependent formulations. Multiple local minima, convergence instabilities and flipping of solutions pose significant difficulties for nonadiabatic molecular dynamics, particularly in the vicinity of ground-state conical intersections[1].

In this work, we build on recently developed Convex Hartree-Fock theory[2], in which the electronic energy minimisation problem is reformulated as a convex optimization over a subspace defined by physically motivated constraints. By construction, the convex Hartree-Fock (CVX-HF) framework admits a unique minimum, eliminating SCF instabilities and providing smooth, well-defined energy surfaces across nuclear configurations (see Fig.1). This reformulation enables robust optimization using modern convex solvers and eliminates the need for manual intervention near degeneracies, paving the way for autonomous molecular simulations in challenging regions of configuration space.

We further introduce convex Density Functional Theory (CVX-DFT), a natural extension of the convex framework to DFT that preserves its favourable scaling and accuracy while avoiding pathological behaviour near degeneracies. CVX-DFT goes substantially beyond the current state of the art and will allow stable excited-state dynamics and nonadiabatic simulations that remain well-behaved around conical intersections, a long-standing bottleneck for photochemistry, and establishes a foundation for the development of new density functionals that accurately capture nonadiabatic regimes.

Beyond methodological robustness, convex formulations also improve reproducibility and facilitate AI-assisted or fully autonomous workflows. CVX-HF and CVX-DFT thus represent a promising direction for next-generation quantum chemical methods that couple rigorous optimization with automated simulation, supporting reliable molecular dynamics for complex chemical systems.

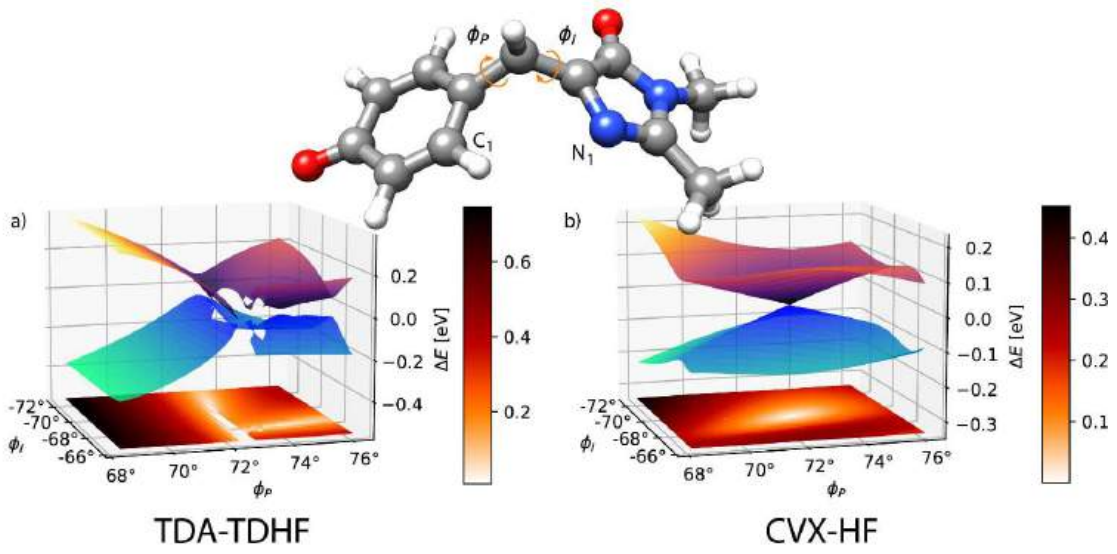

Fig. 1. Comparison of TDA-TDHF (a) and CVX-HF (b) potential energy surfaces of S_0 and S_1 in $HBDI^-$, the chromophore for the Green Fluorescent Protein (GFP). The geometry at the CVX-HF CI is shown in the middle. The energies are relative to the average energy of the states. At the bottom of each plot, a colormap shows the value of $E_1 - E_0$ in eV.

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CAI - D3 - O04
Computational modeling of tryptophan fluorescence spectra in proteins

Federica Borzelli[1], Alessio Olivieri[1], Andrea Amadei[2], Marco D'Abramo[1]
[1]Sapienza University of Rome, Italy; [2]University of Rome Tor Vergata, Italy

Protein fluorescence is dominated by tryptophan, whose electronic transitions feature a large transition dipole and strong sensitivity to the local environment, making it a useful probe for ligand binding and conformational changes. However, assigning spectral features is challenging when multiple tryptophans contribute to emission.
Here, we adopt a theoretical-computational method to predict fluorescence spectra and maximum wavelengths (λmax) in proteins. The approach relies on the Molecular Dynamics–Perturbed Matrix Method (MD-PMM), a QM/MM technique combining extensive MD sampling with QM calculations at moderate computational cost. Building on a previous application to indole in water[1], we extend the approach to indole in proteins. QM electronic properties are computed for a selected quantum center (QC), the indole moiety of tryptophan, in gas-phase. MD simulations of the full system are performed using ESP charges of the bright excited state, to sample conformations representative of the emitting ensemble. From the MD simulations, we evaluate the environment perturbation to the QC Hamiltonian, yielding excitation energies in a realistic environment. The emission spectrum is obtained from the resulting distribution of vertical transition frequencies and transition dipoles; vibronic structure is included by evaluating the vibrational eigenstate overlap between the ground and excited electronic states.
We tested the approach on AlbAS, an eight-tryptophan protein, obtaining spectra for eight single-tryptophan mutants. While predicted λmax resulted slightly blue-shifted relative to experiment[2], they reproduced the expected red-shift from apolar to polar environments around tryptophan. Ongoing work is validating the method on additional proteins with experimentally characterized fluorescence spectra, with the goal of providing a practical tool to support assignment of emission maxima in multi-tryptophan systems.

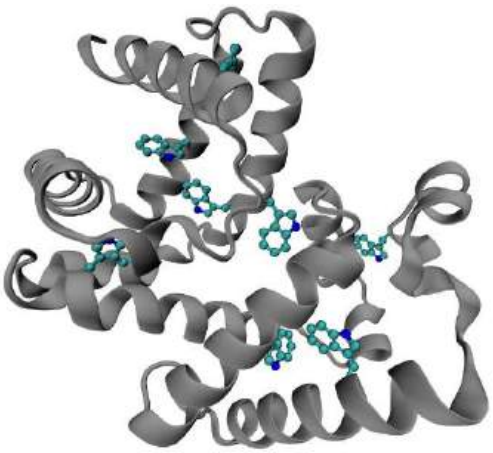

Figure 1. Representation of the AlbAS protein (PDB: 6ET8). The eight tryptophan residues are highlighted.

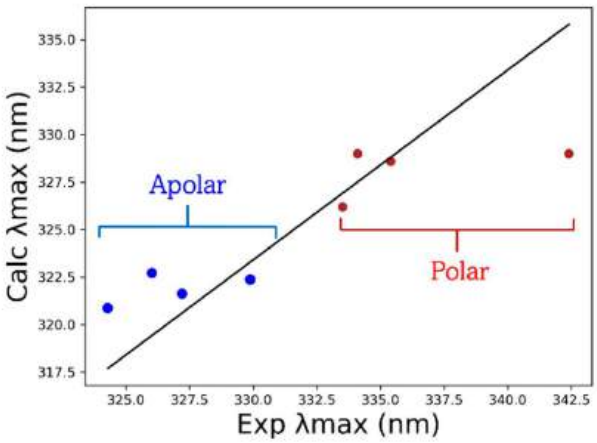

Figure 2. Linear fit of experimental and preliminary MD-PMM computed λmax for eight single-tryptophan mutants of the AlbAS protein.

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CAI - D3 - O05
Organic diradicals bridged by inverted singlet-triplet units for optical-spin interfaces

Lorenzo Savi[1], Marco Tommaso Barreca[1], Matteo Bedogni[1], Francesco Di Maiolo[1]
[1]*Dept. of Chemistry, Life Science and Environmental Sustainability, University of Parma, Italy*

Molecular platforms for optically addressable spin states are emerging as fascinating alternatives to solid-state spin centers, offering scalable synthesis, structural tunability, and chemical versatility.[1-4] In this talk, we present a molecular design strategy for achieving photoinduced spin polarization in organic diradicals bridged by systems featuring an inverted singlet-triplet (InveST) energy gap (see **Error! Reference source not found.**).[5] These InveST units possess HOMO and LUMO orbitals localized on complementary atomic sites. By covalently linking the non-SOMO-bearing positions of alternant hydrocarbon radicals to the LUMO-localized atoms of the InveST bridge, we construct diradicals in which the radical centers remain electronically decoupled in the ground state, yielding degenerate singlet and triplet configurations. Upon photoexcitation, population of the InveST LUMO activates an excited-state exchange interaction between the radicals, generating a finite singlet-triplet gap and enabling spin-selective intersystem crossing to polarized triplet states. Using a combination of model Hamiltonians and multireference *ab initio* calculations, we establish design principles for tuning exchange interactions and spin-orbit coupling to achieve molecular-level control over optical-spin interfaces. The resulting InveST-bridged diradicals emerge as promising scaffolds for molecular quantum technologies.

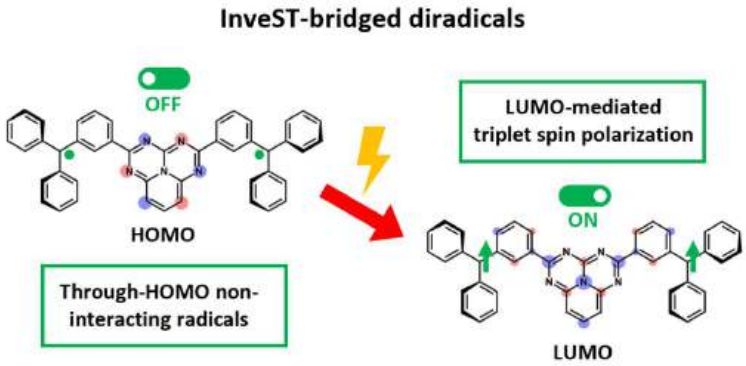

Fig. 1. Schematic overview of the InveST-bridged diradical design and of the spin-spin locking as induced by the InveST-localized HOMO→LUMO transition.

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CAI - D3 - O06
Data-driven prediction of spin-crossover properties from electronic structure calculations

Laia Navarro[1], Arnau Garcia-Duran[1], Jordi Cirera[1]
[1]Dept. de Química Inorgànica i Orgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Spain

Spin-crossover (SCO) compounds are transition-metal complexes in which the electronic spin state of the metal ion can be reversibly switched between low-spin and high-spin configurations using an external stimulus, such as temperature, pressure, or electromagnetic radiation. This phenomenon originates due to the balance between ligand-field splitting and electron pairing energy, producing drastic changes in magnetic, optical, and structural properties. Because of their intrinsic switching behavior, SCO materials are perfect candidates for nanoscale-based applications, including molecular electronics and data storage.
For thermally induced SCO systems, the temperature with equal populations of both spin states is defined as the transition temperature ($T_{1/2}$), a key parameter in their physical characterization. However, $T_{1/2}$ remains difficult to predict experimentally, making computational approaches a powerful tool for the design of new SCO materials.[1,2] In this work, we will show how density functional theory (DFT) calculations can quantitatively reproduce experimental $T_{1/2}$ values for different families of SCO compounds. These methods enable the exploration of higher nuclearity systems or less common metal ions, such as $[Cr^{II}(Tpm^{R})_2][BF_4]$ (Tpm = tris(pyrazolyl)methane) or $[Mn^{III}(OL_1)_2]Cl$, (OL_1 = (2-pyridyl) (2-pyridylamino)methanolate).[3,4]
Electronic structure calculations allow for a systematic *in silico* exploration of the ligand chemical space, explaining how inductive, resonant, and steric effects interplay to modulate the ligand field strength and, therefore, the associated $T_{1/2}$ trends. Furthermore, due to the high accuracy of our DFT results, we constructed datasets to train machine learning models capable of automatically classifying Fe(III) compounds into high-spin, low-spin, or spin-crossover categories.[5] When combined with Graphic Process Units (GPUs), this approach enables efficient virtual screening and recovery of novel SCO molecules, as we did for the $[Fe(phen)_2(NCS)_2]$ family. Thus, this work provides with guidelines for the rational design of new SCO materials with targeted $T_{1/2}$, based on the underlying electronic structure in terms of the relevant d-based molecular orbitals.

J.C. thanks the Spanish MICINN research grant (PID2023-146774NB-I00). J.C. and A. G-D the Spanish Structures of Excellence María de Maeztu program (CEX2021-001202-M). A. G-D is grateful for an FPI grant (CEX2021-001202-M)

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CAI - D3 - O07
Digital twins to design reactors for efficient photochemistry

Jasper H. A. Schuurmans[1], Timothy Noël[1]
[1]*Universiteit van Amsterdam (UvA), The Netherlands*

Photochemistry has become integral to modern synthetic chemistry, enabling transformations that are inaccessible under conventional conditions. Despite the widespread use, photochemical reactor designs vary considerably between laboratories. Lab-scale reactors are typically 3D-printed, introducing flexibility and accessibility, but also leading to the introduction of numerous different interpretations and reactor designs.[1] Intuitively finding the optimal reactor for each case study is challenged by the complexity of the interactions of light.[2] Whereas optimization is rarely performed due to the high time investment and costs related to the experimental work. Light interactions can be described with ray-tracing, allowing for the formation of virtual representations of reactor setups, so called digital twins. These models can be exploited for rapid characterization of light intensity and photon flux, leading to quick gathering of data.
This reliable data, when combined with machine learning tools, can be used to design reactors that utilize light sources more efficiently, potentially accelerating photochemical reactions. In addition, the use of simulations facilitates the photonic characterization of reactors and enables straightforward quantum yields studies. In our work, we investigate a photocatalytic Suzuki-Miyaura cross-coupling reaction between an aryl bromide and triethylborane using an optimized photoreactor. The interplay between photochemical steps and the nickel catalytic cycle, and its effect on the apparent quantum yield was investigated by varying, the photocatalyst, ligands, and nickel concentration. Overall, we propose a robust framework that synergistically couples digital twins with machine learning to achieve more energy-efficient and accelerated photochemical processes.

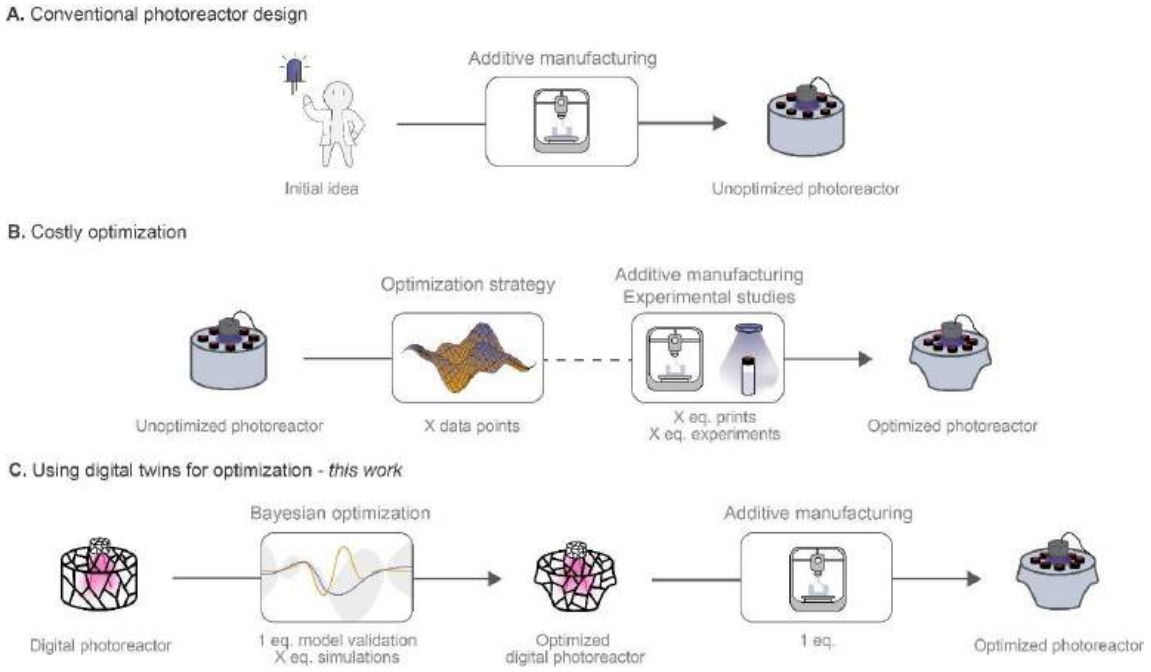

Fig. 1. A. Conventional pathway for the design of photoreactors, often based on intuition. B. Optimization is rarely performed, as it requires costly experimental work. C. The use of digital twins replaces experimental work with simulations, leading to a swift optimization process.

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CAI – D3 - O08

Chiral deep eutectic solvents as catalysts for asymmetric synthesis: A machine learning–driven molecular dynamics design tool

Michele Tomasini[1], Matteo Tiecco[2] , Diego A. Alonso[3], Laura Falivene[1]
[1]Dept. di Chimica e Biologia, Università di Salerno, Italy; [2]Chemistry Interdisciplinary Project (ChIP), School of Pharmacy, University of Camerino, Italy; [3]Dept. de Química Orgánica, Facultad de Ciencias, and Instituto de Síntesis Orgánica (ISO), Universidad de Alicante, Spain

Deep eutectic solvents (DESs) have emerged as promising, sustainable alternatives to traditional organic solvents in catalysis, owing to their tunable properties, low toxicity, and environmental friendliness. While DESs have demonstrated potential as reaction media for organocatalytic processes, their catalytic activity remains less understood. The role of DESs as catalysts themselves is an area of growing interest, but the intricate interactions between the DES components and catalytic systems require a deeper understanding to harness their full potential.

This study utilizes Molecular Dynamics Simulations using Machine Learning Interatomic Potentials[1] as an indirect but powerful method to understand the catalytic behavior of DESs in organocatalytic reactions.

We focus here on the catalytic activity and stereoselectivity of DESs in model Michael additions, where DESs are shown to exhibit catalytic properties via hydrogen-bonding networks and other non-covalent interactions. Calculations provide detailed insights into how these solvents influence reaction pathways and enhance selectivity.

Specifically, this works aim to probe the electronic structure of DESs for systems containing L-proline[2] and novel chiral (ammoniummethyl)pyrrolidine-derived hydrogen bond acceptor[3], to compare and understand the influence of DES strcuture on the catalytic activity.

Analysis of radial distribution functions from the molecular dynamics trajectories allowed us to pinpoint the hydrogen-bond interactions within the DESs and to establish a clear link between their strength and nature and the observed catalytic performance.[4] These insights provide a molecular-level framework to rationalize how the interplay between hydrogen-bond donors and acceptors controls the organocatalytic behaviour of chiral eutectic mixtures, paving the way toward the predictive design of next-generation DESs for asymmetric catalysis.

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CAI - D3 - O09

Formation of oxynitrides under ambient condition during post-deposition process: An ab initio molecular dynamics study on the oxidation process of metal nitrides

Ji Liu[1], Michael Nolan[1]
[1]*Tyndall National Institute, University College Cork, Ireland*

The surface N of transition metal nitride can be a solution to nitrogen reduction reaction with initial N vacancy formation via hydrogenation steps and ammonia formation. We have successfully deposited VN[1] and ZrN[2] films using metal organic chemical vapor deposition method with new single-source precursor and these deposited metal nitride thin films rapidly oxidizes when exposed to ambient conditions and forms metal oxynitrides species on the surface.
In this presentation, I will discuss in detail with aiMD the unintentional oxidation of ZrN and VN surfaces by oxygen present at ambient conditions[3] at various temperatures. Results show that ZrN surfaces tend to form oxynitrides at lower temperatures and prefer to form a ZrOx layer interfaced with ZrN at higher temperature. VN(111) forms VO_x clusters on the surface, and there is no significant migration of the O species into bulk VN at all studied temperatures. We attribute the different oxidation processes of ZrN and VN to the relative strengths of V–N/O bonds and Zr–O/N bonds─the bond dissociation energy of V–N (452 kJ/mol) is larger than that of Zr–N (339 kJ/mol), while the V–O bond (645 kJ/mol) is weaker than the Zr–O bond (776 kJ/mol). Experimental results on MOCVD nitride films confirm that VN is less oxidized than ZrN at ambient conditions because VN forms a less stable, potentially volatile oxide layer, whereas ZrN has a stronger tendency to form a stable, protective ZrO_2 layer, promoting more complete oxidation at higher temperatures. This study defines a new degree of atomic-scale understanding of the formation of oxynitride at ambient oxygen conditions relevant for NRR electrocatalysis.

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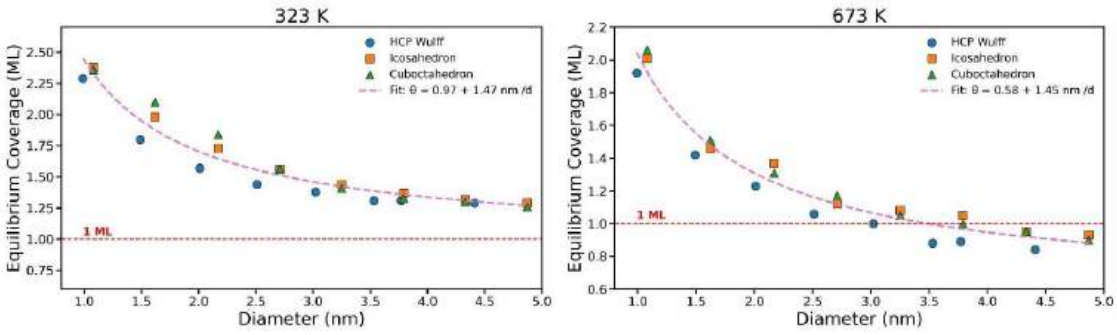
CAI - D3 - O10

Multiscale modeling of hydrogen coverage on Ru nanoparticle: A combined DFT, AIMD, and DPMD study

Wenye Xuan[1], Yu-Hao Liu[1] and Hsin-Yi Tiffany Chen*[1-3]

[1]Dept. of Engineering and System Science; [2]Dept. of Materials Science and Engineering; [3]College of Semiconductor Research, National Tsing Hua University, Taiwan

Ruthenium (Ru) nanoparticles excel in thermal catalytic hydrogenation reactions like ammonia synthesis, but suffer from hydrogen poisoning, where strong H chemisorption blocks reactant adsorption. Experimentally, Ru particle size and dispersion are commonly determined via hydrogen adsorption, employing an assumed 1 ML coverage as reference, disregarding the effects of size, morphology, and operating conditions on hydrogen adsorption behavior. In our recent studies, we employed a multiscale framework integrating density functional theory (DFT), ab initio phase diagrams, ab initio molecular dynamics (AIMD), and deep potential MD (DPMD) to predict the stable morphologies of 1–10 nm Ru nanoparticles and their detailed hydrogen adsorption behaviors. Our melting simulations and analyses revealed that stable morphology of Ru nanoparticles exhibits a size-dependent transition: icosahedral morphology is preferred below 1 nm, decahedral between 1–5 nm, and HCP above 5 nm.[1] Hydrogen adsorption predictions reveal >1 ML coverage, especially for small particles: ~2.4 ML at 1 nm and ~1.3 ML at 4.8 nm (323 K, DPMD), dropping to ~2 ML, ~1 ML, and ~0.9 ML at 673 K.[2] Notably, our simulations demonstrated that hydrogen coverage scales with low-coordinated surface Ru atoms that dominate at nanoscale. Consequently, hydrogen coverage does not linearly scale with Ru nanoparticle size, challenging common assumptions in hydrogen adsorption studies. Specifically, hydrogen adsorption experiments to characterize Ru nanoparticles can lead to overestimated dispersion and underestimated size. We herein propose a new equation to correctly correlate hydrogen adsorption with Ru nanoparticle size: $\theta(d) = a + b/d$ where, θ is the hydrogen coverage, and d is the particle diameter, while a and b are temperature-dependent constants. This new framework bridges scales, challenges idealized models and assumptions, and offers insights into supported Ru nanoparticle catalysts, transferable to other nanocatalysts, guiding their further materials design and development.



The authors acknowledge National Science and Technology Council, NSTC (114-2223-E-007-017-MY5, 114-2112-M-007-041, 114-2124-M-007-007, and 114-2923-E-008-002) in Taiwan for financial supports and thank the computational resources provided by the National Center for High-Performance Computing (NCHC), Taiwan, and the University of Liverpool Barkla HPC cluster.

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CAI - D3 - O11

Computational study of N-methylacetamide (NMA) amide bond cleavage reaction in neutral and alkaline conditions

Edoardo Panzetta[1], Massimiliano Aschi[1], Marco D'Abramo[2]
[1]University of L'Aquila, Italy; [2]Sapienza University of Rome, Italy

The peptide bond has crucial role in chemistry of proteins, since its nature regulates different biochemical processes. Although peptide bonds are very stable under physiological conditions, their cleavage can be accelerated by orders of magnitude by acting on temperature and pH. To date, few publications have been reported in the literature. In this study, we apply a computational approach able to reconstruct the free energy profile of this reaction and the associated kinetic constants under alkaline and neutral conditions, to better understand the mechanism and the influence on the overall kinetics of the process[1,2]. That is, we apply the Perturbed Matrix Method (PMM), a theoretical-computational QM-MM approach that considers a system divided into two parts: the quantum center, treated with quantum mechanics calculations and the environment, treated with classical Molecular Dynamics simulations. Our work began with the study of a small model system with an amide bond to represent the peptide bond, N-methylacetamide (NMA), thus neglecting the presence of amino acids' lateral chains and conformational effects present in proteins. By means of PMM, we modelled the entire mechanism of the reaction, in both conditions, and estimated the reaction kinetics at 360 K, through Eyring equation. Our results are, for the reaction in alkaline condition, in agreement with literature data[3] and initial experiments; the reaction studied in neutral condition doesn't permit an experimental comparison due to the very slow half-time (years). Next steps will be studying larger systems with different amino acid compositions, to understand the role of flanking peptides as well as of the side chains on the kinetics of this reaction.

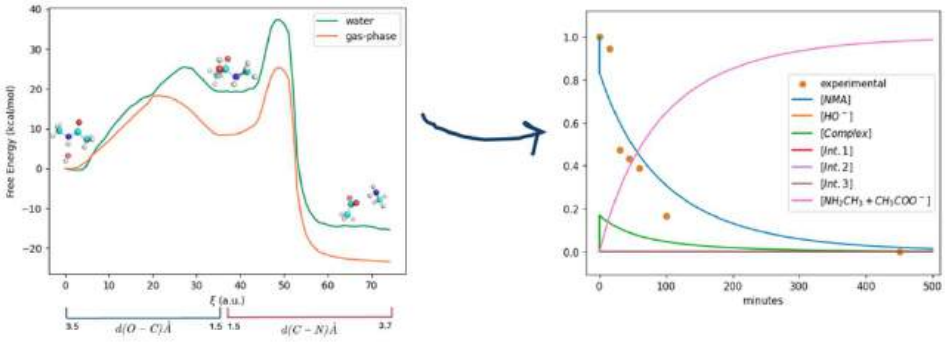

Fig. 1. Unperturbed and perturbed free energy profiles of reaction (left) and comparison between computational and experimental data (right); both figures represent the reaction at alkaline pH.

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CAI - D3 - O12

A computational study of beta cyclodextrin-based nanosponge inclusion complexes

Giulia Ciattaglia[1]*, Marco D'Abramo[1], Sergio Moya[2], Paolo Di Gianvincenzo[2]
[1]Sapienza University of Rome, Italy; [2]CIC biomaGUNE, Spain

β-Cyclodextrins (β-CDs) are cyclic oligosaccharides characterized by a hydrophilic surface and a hydrophobic inner cavity. Due to their non-toxicity and their ability to interact with a wide range of hydrophobic molecules, they are used in several fields, from pharmaceutical to environmental sector[1]. In this study, we firstly investigated the binding behavior of β-cyclodextrin with several guest molecules, such as drugs and pollutants, by means of molecular dynamics simulations. The thermodynamic[2] and structural investigation of these complexes highlighted a reversible and stable inclusion mechanism, suggesting that β-CDs-based systems may represent promising materials for both drug delivery and for the removal of environmental pollutants. Building on these results, we propose a computational study of a β-CD-based nanosponge (EPCN) in which individual β-CD units are crosslinked by epichlorohydrin molecules. The most challenging aspect of this work was the parametrization of the nanostructure, since no suitable data were available in literature. After successfully constructing and parametrizing the EPCN structure, we started investigating its interaction with two drug molecules, doxorubicin (DOXO) and *N*,*N*-bis (5-ethyl-2-hydroxybenzyl) methylamine (EMD)[3], by means of molecular dynamics simulations. An analogous investigation will be carried out for EPCN interactions with pollutant molecules.

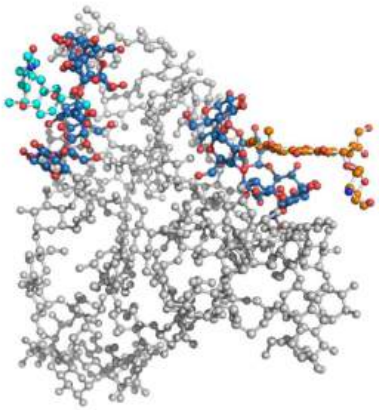

Fig. 1. Representation of EPCN structure interacting with EMD and DOXO drugs.

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CAI - D3 - O13
From mechanisms to function: Computational studies of peptide self-assembly at interfaces

Torsten John[1,2]
[1]Constructor University, Germany; [2] Max Planck Institute for Polymer Research, Germany

Understanding and controlling peptide self-assembly is a central challenge in biophysical chemistry, with implications ranging from pathological aggregation to functional biomaterials. A core focus of our group is the use of molecular dynamics (MD) simulations, integrated with experiments, to establish mechanistic and predictive links between peptide sequence, environment, and emergent structure. We investigate peptide self-assembly both in solution and in the vicinity of biomolecular interfaces, where aggregation frequently occurs under physiological conditions. MD simulations of the amyloid-forming peptide GNNQQNY resolve competing fibril growth pathways, revealing monomer surface diffusion towards fibril ends as a dominant elongation mechanism, alongside lateral association of protofibrils into higher-order assemblies.[1] A second research axis addresses peptide-membrane interactions as modulators of self-assembly. Simulations and experiments using model membranes with varied lipid composition, including oxidized lipids, demonstrate how electrostatics, surface attraction, and secondary-structure stabilization determine whether membranes accelerate or inhibit aggregation in a peptide-specific manner.[2] This framework provides predictive insight into how changes in membrane chemistry influence aggregation pathways in biological environments. Building on these mechanistic insights, we pursue sequence-guided design strategies for functional peptide fibrils, exemplified by neurotrophic peptides derived from enhancing factor C, where hydrophobic core design controls fibril stability and bioactivity.[3] Our work aims to integrate MD, structure prediction, and experimental feedback into unified workflows for the rational design of peptide-based biomaterials and biointerfaces.

The presented studies build on collaborations with the co-authors of the cited publications.

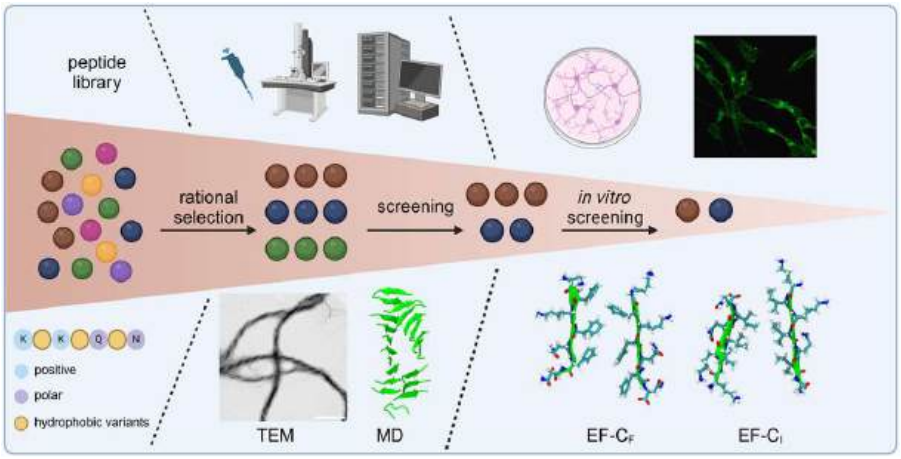

Fig. 1. Workflow of peptide fibril materials design.[3]

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CAI - D3 - O14

Programmable peptide–graphite interfaces for water bioremediation: From Gly–X sequence to ion capture

Horacio Poblete[1], Eduardo Cubillos-Llantén[1], Jeffrey Comer[2]
[1]Universidad de Talca, Chile; [2]Kansas State University, USA

Phosphate and nitrate are hard to remove from water because they dissolve easily and interact only weakly with most materials. Graphitic surfaces can guide how cyclic Gly–X repeat peptides fold and align, creating ordered, sequence-programmable nanointerfaces for selective capture.[1],[2] Yet current sorbents seldom use sequence to control interfacial structure, and we still lack a quantitative map connecting cyclic-peptide sequence, graphite-templated folding/assembly, and oxyanion binding.

Here, we design cyclic Gly–X repeat scaffolds with compact, symmetric turns that promote flat β-hairpins and in-register assembly on graphite.[1]–[3] Using large-scale molecular dynamics, replica-exchange umbrella sampling to resolve folding and registry, and alchemical free-energy calculations (FEP) to parse residue-level contributions, we quantify structural stability and binding of phosphate and nitrate at preorganized motifs.

Four findings stand out. First, templated folding: Gly–Thr repeats with symmetric GPGG turns display a deep folded minimum on graphite and suppress out-of-register states versus solution. Second, cooperative assembly: hairpins extend into planar β-sheet arrays; breaking loop symmetry or lengthening strands increases frustration and defects. Third, crowding-dependent cooperativity: as peptide surface density rises, intermolecular contacts stabilize arrays built from small side chains (Gly, Ala), while bulkier/polar Thr shows reduced cooperativity under crowded conditions—an effect captured by FEP as enhanced stabilization for Gly/Ala and diminished gains for Thr. These results indicate that intermolecular interactions promote stabilization for small side-chain residues such as Gly and Ala, while bulky or polar groups like Thr show reduced cooperativity under crowded conditions. Fourth, selectivity and energetics: periodic grooves in the assembled monolayers preposition hydrogen-bond donors and electropositive patches that favor oxyanion adsorption; sequences that balance short Gly–X strands with high-fidelity registry enhance phosphate binding over nitrate.

In sum, cyclic Gly–X repeat peptides on graphite turn sequence into function: surface-templated folding and density-dependent cooperativity enable selective, water-compatible capture of phosphate and nitrate—yielding actionable design rules (symmetric GPGG turns, short-to-medium Gly–X strands, planar monolayers). These insights guide our next step: introducing charged noncanonical residues into short repeats to optimize both folding and anion adsorption for programmable bioremediation interfaces.

Acknowledgements: FONDECYT-Chile Grant 1251288

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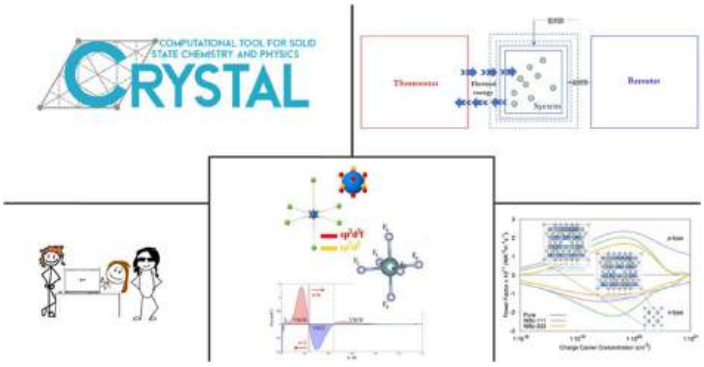
CAI - D3 - O015
CRYSTAL, an ongoing project for a theoretical chemical approach to solids

Silvia Casassa[1], Chiara Ribaldone[1], Andreha Gelli[1,2]
[1]University of Turin, Italy; [2]Universitat Autònoma de Barcelona, Spain

CRYSTAL is a quantum mechanics program for studying the chemical and physical properties of materials.[1] This research project began 50 years ago thanks to the initiative of three scientists from Turin, and has grown with the collaboration and contributions of researchers from across Europe. The project continues to grow thanks to the transfer of skills and passion to new generations of young researchers who advance it with new visions, sensibilities and expertises.
In this context, it is important to emphasize that the CRYSTAL code approaches the study of materials with an eminently chemical attitude: it uses a basis set of atomic orbitals to describe the wave function and is able to model molecules, polymers, and surfaces, as well as bulk materials, with the same degree of accuracy and correct dimensionality (i.e. without replicas).
This is an opportunity to present some of the code's latest developments, which expand its potential and enable even closer and more fruitful interaction with the experimental counterpart.
The following topics will be covered:

- A module for the study of nuclear motions: molecular dynamics[2] (NVE, NVT, and NPT) and nudged-elastic band method[3] (NEB) implementations to study transformations on different time scales, including the effects of temperature and pressure.
- Techniques to perform the topological analysis of the electron density according to Bader theory, capable of recognizing atoms within crystals and providing information on their bonding properties.[4]
- Calculation of electronic conductivity and associated properties[5] (Seebeck effect) and initial development of a method to reproduce electron-phonon coupling.



These aspects will be illustrated from a formal perspective, and for each of them, relevant tests and applications will be presented to support the increasingly pressing need to combine experimental chemistry with theoretical study.

Acknowledgements: The perspectives I will outline, as well as the results presented, are primarily the result of the work of the two young co-authors, whom I thank for their enthusiasm, passion, and professionalism, without which Science would not be possible.

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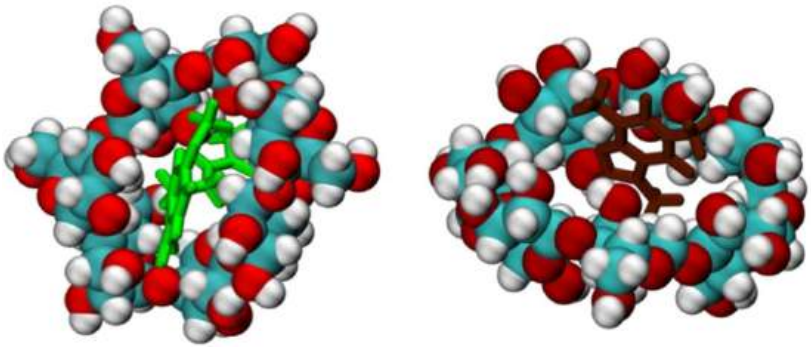
CAI - D3 - O16
Multiscale approaches to drug encapsulation and release in β-cyclodextrin-based systems

Marta Corno[1], Sofia Chiara Sarnataro[1], Massimo Delle Piane[2], Valentina Brunella[1]
[1]Dept. of Chemistry, University of Turin, Italy; [2]Dept. of Applied Science and Technology, Politecnico di Torino, Italy

Cyclodextrin-based drug delivery systems are widely regarded as versatile supramolecular platforms, owing to their ability to encapsulate chemically diverse guest molecules and to modulate drug stability and release kinetics. Melatonin (MT) is a particularly relevant target for cyclodextrin encapsulation, due to its rapid clearance and limited bioavailability.
In this contribution, we present a multiscale computational framework to support the rational design of CD-based carriers by elucidating the structural, energetic, and kinetic determinants of host–guest complexation. The approach integrates quantum mechanical calculations, classical molecular dynamics, and enhanced sampling techniques to explore both molecular recognition and nanoscale organization in cyclodextrin systems.
At the molecular level, the conformational landscapes of native α-, β-, and γ-cyclodextrins were systematically investigated through a hierarchical protocol combining semi-empirical conformational sampling with composite density functional theory optimizations.[1] An automated workflow was developed to generate libraries of derivatized CDs and systematically evaluate their inclusion complexes with melatonin and selected guest molecules.[2]
The approach was extended to a diverse set of model drugs and small gas molecules, and to larger-scale cyclodextrin nanosponge models investigated through microsecond molecular dynamics simulations in explicit solvent.[3] Enhanced sampling via metadynamics provided access to free energy profiles and kinetic parameters of encapsulation and release processes, offering mechanistic insight beyond static binding geometries.
Overall, the resulting multiscale dataset establishes a robust computational foundation for understanding and tuning cyclodextrin-based drug delivery systems, highlighting the central role of modeling in guiding the design of supramolecular nanocarriers with tailored loading and release properties.



Optimized inclusion complexes of β-cyclodextrin with melatonin (left) and caffeine (right), illustrating the host–guest arrangement within the cyclodextrin cavity. Color code: oxygen atoms in red, hydrogen in white, carbon in light blue; melatonin is shown in green and caffeine in brown.

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CAI - D3 - O17
Including charge transfer states in fragment based exciton calculations

Bónis Barcza[1,2], Attila Tajti[2], Péter G. Szalay[2]
[1]ELTE Eötvös Loránd University, Hevessy György PhD School of Chemistry, Hungary; [2]ELTE Eötvös Loránd University, Institue of Chemistry, Hungary

Charge transfer (CT) states pose a large hurdle for multilevel methods, especially when the electron leaves the active center. Since embedding/fragment approaches are crucial for large systems, there is an urgent need to incorporate not just local, but also CT excitations in these procedures. We aim to develop a framework that can treat these states and their interactions on an equal footing without compromising the accuracy of the high-level method while keeping the computational cost low.
The method we suggest is the generalization of the excitonic fragment method in Ref. 1. In this approach the Hamiltonian is diagonalized in the space of the local excited states of the dimer: diagonal elements are the energy of them, while off-diagonal elements represent the coupling between these. Now interfragment CT states need to be included, which dissociate into two ions. The couplings among them and the valence states need to be considered as the off-diagonal elements of the Hamiltonian. These can be evaluated using the toolset of second quantization, which was designed to treat both Coulomb and exchange-type contributions, with variability regarding the electron number. The biggest theoretical challenge is that the wavefunctions of the subsystems overlap, complicating the description considerably. We solved this problem by applying the transformation presented in Ref. 2. By construction, we get Coulomb and exchange terms, for each type of interaction: local-local (Frenkel), CT - CT and CT-local terms as well.
Our results show that the suggested technique indeed accounts for CT effects appropriately and can describe the excited state potential energy curves across a wide range, for reasonable computational cost. Moreover, the local-CT coupling was found to be important, if present, it dominates the interaction between the states affecting the potential curves considerably. Accuracy-wise, we were able to achieve close to supersystem coupled cluster (CC) level by data only from monomers described on the same CC level. Generalization to more fragments is also possible opening a new avenue for high-accuracy quantum chemistry of the excited states of large systems.

This work has been supported by the National Research, Innovation and, Development Fund (NKFIA) of Hungary, Grant No. 142634. BB acknowledges the support and funding from the DKOP-23 doctoral excellence program of the ministry for culture and innovation from the source of the national research, development and innovation fund.

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CAI - D3 - O18

DFT insights into GaSe/InS Heterostructures for visible-light-driven water splitting with high solar-to-hydrogen efficiency

Shang-Hao Chiang[1*], Chen-Hao Yeh[1]
[1]Dept. of Materials Science and Engineering, Feng Chia University, Taiwan

Due to the escalating environmental threats posed by fossil fuels, the pursuit of alternative energy sources has become increasingly urgent. Hydrogen energy has emerged as a promising solution, with photocatalytic water splitting recognized as a clean and sustainable method for hydrogen production. Among recent developments, two-dimensional (2D) heterostructures have attracted significant attention for their enhanced photocatalytic properties, such as narrowed band gaps and efficient charge separation. In this study, we employed density functional theory (DFT)[1] to investigate novel 2D heterostructures[2] [3] based on group-III monochalcogenides, focusing primarily on the GaSe/InS system. Our calculations reveal that all considered heterostructures possess band gaps exceeding 1.23 eV, and notably, GaSe/InS exhibits a favorable type-II band alignment. Optical absorption analysis indicates strong visible-light activity in the 380–760 nm range. Furthermore, we calculated Gibbs free energy curves, three different paths of oxygen evolution reaction (OER) were considered, the results shows that the InS monolayer effectively facilitates in OER-III, while GaSe is more suitable for the hydrogen evolution reaction (HER), exhibiting a low free energy change. Last, the GaSe/InS heterostructure demonstrates a promising solar-to-hydrogen (STH) efficiency of 32%. This results again proofs that 2D GaSe/InS heterostructure is a suitable material for photocatalysis water splitting.

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CAI - D3 - O19
Recent progress in computational Auger spectroscopy

Thomas Jagau[1]
[1]*Dept. of Chemistry, KU Leuven, Belgium*

The emission of an Auger electron is the predominant relaxation mechanism of core-vacant states in molecules composed of light nuclei. In this non-radiative decay process, one valence electron fills the core vacancy, while a second valence electron is emitted into the ionization continuum. Although Auger spectroscopy is well established as an analytic technique for molecules, surfaces, and solids, the theoretical modeling of molecular Auger spectra from first principles remains challenging. This pertains in particular to advanced techniques that rely on coincidence measurements of several Auger electrons, probing their relative energy or orientation.
In this contribution, I will review the progress achieved in this field over the past few years. Based on non-Hermitian quantum chemistry, we have been able to construct regular and resonant Auger spectra for 1s, 2s, and 2p ionization edges of various molecules including benzene and thiouracil. I will also discuss which developments are needed to model processes such as double Auger decay that are still largely beyond the reach of state-of-the-art quantum chemistry.

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CAI - D3 - O20

Seamless integration of machine-learned interatomic potentials into quantum chemistry workflows with ChemRefine

Alistair J. Sterling[1]
[1]*The University of Texas at Dallas, United States*

Machine learning is playing an increasingly important role in computational chemistry, with the promise of accelerating routine tasks while enhancing the accuracy of predictions. A major challenge, however, lies in connecting newly developed machine-learned interatomic potentials (MLIPs) with existing quantum mechanics (QM)-based workflows that remain central to the field. To address this gap, we introduce ChemRefine, an open-source modular automation platform designed to seamlessly integrate the next generation of MLIPs into computational chemistry pipelines.[1] ChemRefine is built to operate flexibly across a wide spectrum of research tasks including conformational sampling, host–guest binding studies, redox and photophysical property prediction, transition state finding, molecular dynamics spawning, and microsolvation. Beyond executing these tasks, ChemRefine can train, fine-tune and deploy MLIPs during the course of a workflow, allowing researchers to accelerate their calculations without compromising accuracy. We will demonstrate the utility of ChemRefine through vignettes of recent and ongoing projects from our group that rely on automation and mixed quantum/machine learning workflows.[2]

This work was supported by the ACS Petroleum Research Fund (69496-DNI), the NVIDIA Academic Grant Program, and start-up funding from The University of Texas at Dallas.

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CAI - D3 - F01
Automated design of peptide-based scavengers using MLIPs and Boltz2

Lucia Warner[1], Mauricio Cafiero[1]
[1]University of Reading, UK

Variable length peptides are designed to scavenge organic UV filters used frequently in sunscreen formulations. Multiple of these molecules are typically used in sunscreens to offer broad protection across UVA and UVB rays[1], however this comes at an environmental cost. Alongside harm to aquatic life, these UV filters have been shown to cause coral bleaching. Scavenger peptides designed specifically to bind these molecules may offer an environmentally friendly way to reduce their impact. We have developed a model that generates various conformations of a defined set of amino acids and places them in random poses around the UV filter molecule in question. The model then uses a Machine-Learned Interatomic Potential (MLIP)[2] to evaluate each pose and saves any below a certain threshold. Promising poses for each amino acid are further optimized in explicit solvent using the MLIP. The model then combines the most attractive poses for each amino acid into a peptide, adding the appropriate number of spacers (gly) where needed. A mask-filling protein model is used to replace the spacers with appropriate amino acid residues, and the final peptides are co-folded with the UV filter molecules using Boltz2[3], which provides the final binding energy for the peptide. Initial work shows good binding, and experimental testing will be carried out on the generated peptides.

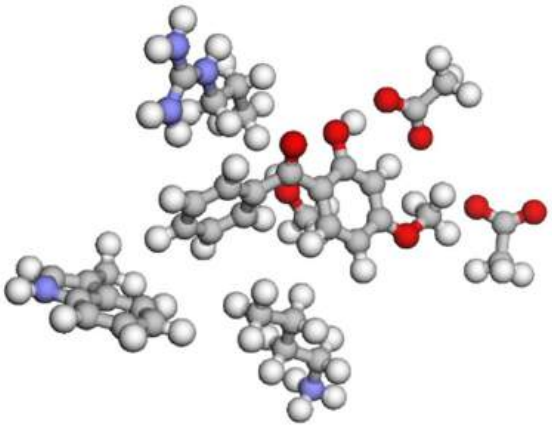

Fig. 1. Intermediate model results: combined residue poses without gly spacers around the UV filter molecule.

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CAI - D3 - F02
Data-driven reactivity design through generative modeling with quantum chemistry validation

Zarko Ivkovic[1,2], Kjell Jorner[1,2]
[1]D-CHAB, ETH Zurich, Switzerland; [2]NCCR Catalysis, Switzerland

Data-driven inverse-design is a new emerging field in chemistry, showing promising results in drug discovery[1,2,3] but remains underutilized in the context of reactivity design. This gap is largely attributed to data scarcity and the lack of generative models explicitly tailored for reaction-centric applications. While existing 3D generative frameworks possess the capacity for conditional generation of molecules, they cannot handle conditional generation on reactive properties, limiting their impact on reactivity design.[4,5] In this work, we present a specialized generative modelling approach aimed at scaffold elaboration for reactivity design. Due to data scarcity, we limit ourselves in this study to reactivity design through scaffold decoration. We construct a curated dataset of around 10,000 DFT-level calculated keto-enol tautomerization reactions by subsampling a combinatorial library sharing a common *N*-Salicylideneaniline core scaffold. We train a 3D structure-generating model on this dataset to produce transition state geometries that exhibit desired reactive properties. The inherent advantage of our approach over existing 2D approaches is easy validation of model predictions due to generated transition states. Our approach demonstrates the potential of targeted scaffold elaboration to advance computational reactivity design and provides a foundation for future developments in structure-based reaction modelling.

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CAI - D3 - F03

Comparative modelling of biological methanation reactors for sustainable CO_2 conversion

Anika Laux[1]*, Miriam Schelle[1], Jiaqi Peng[1], Dominik Engel[2], Carl Fritsch[1]
[1]*Research Institute for Water Management and Climate Future at RWTH Aachen University, Germany;*
[2]*AVT.BioVT Biochemical Engineering, RWTH Aachen University, Germany;*

Biological methanation converts CO_2 and renewable hydrogen into methane, offering a sustainable Power-to-Gas pathway crucial for achieving climate targets[1]. Despite some advantages over catalytic processes, including trace pollutant tolerance and lower operating temperatures, gas-liquid mass transfer limitations remain the primary bottleneck requiring systematic reactor optimization[2].

While individual reactor types have been studied extensively, a unified modelling framework enabling systematic comparative analysis of different reactor configurations has been lacking. This work addresses this gap by developing mathematical models for Continuous Stirred Tank Reactors (CSTR), Bubble Column Reactors (BCR), and Trickling Bed Reactors (TBR).

Models are based on an adapted Anaerobic Digestion Model No. 1[3] with reactor-specific simplifications: TBR assumes plug-flow with explicit biofilm modelling, CSTR assumes ideal mixing, and BCR considers homogeneous flow with gas recycling. Two approaches for volumetric mass transfer coefficient (k_La) calculation were compared: comprehensive correlation-based and simplified empirical methods[4]. The Python implementation with BDF solver showed high agreement with experimental data after calibration of empirical factors, confirming gas-liquid mass transfer as the dominant.

Sensitivity analysis revealed significant reactor-dependent differences: CSTR exhibited the highest sensitivity to maximum substrate uptake rate (8.79×10^3) (see Fig. ***1***) due to biomass dilution at low biological activity. All reactors showed high sensitivity to mass transfer parameters: CSTR to stirring speed (3.06) and impeller diameter (7.76), BCR to recycle ratio (0.486), and TBR to liquid-biofilm mass transfer coefficient (0.792). TBR demonstrated highest pressure sensitivity (0.879) versus CSTR (0.179) and BCR (0.057) (see Fig. ***2***).

Results demonstrate that TBR can be optimized to maximize methane production largely independently of mass and gas transfer rates, while bubble dispersion reactors (CSTR, BCR) exhibit greater operational flexibility at varying hydrogen feed rates - critical for integration with fluctuating renewable energy sources. These insights support optimized reactor selection and process design for sustainable biological CO_2 conversion.

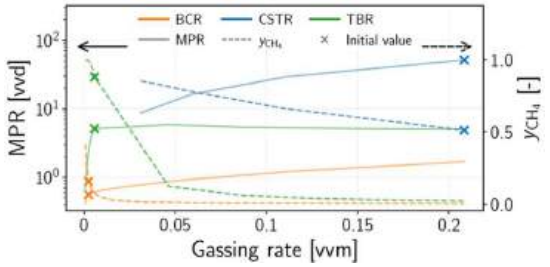

Fig. 1. Sensitivity analysis results showing reactor-specific responses to key parameter maximum substrate uptake rate km,H_2

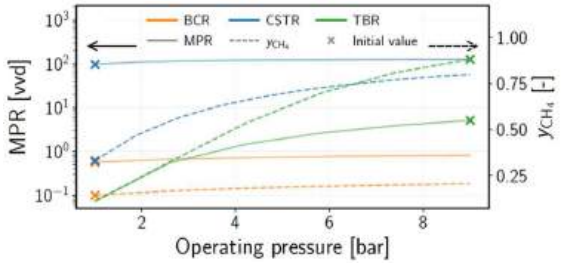

Fig. 2. Sensitivity analysis results showing reactor-specific responses to key parameter operating pressure

This work was conducted within the project "E-MetO", funded by the German Federal Ministry for Economic Affairs and Climate Action under grant 03EI3093B.

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CAI - D3 - F04
Molecular dynamics insights into ion conduction and gating mechanisms of PKD2

Chenfeng Zhang[1], Julien Michel[1]
[1]*University of Edinburgh, UK*

Polycystin-2 (PKD2) is a member of the Transient Receptor Potential Polycystin (TRPP) channel family whose dysfunction is associated with autosomal dominant polycystic kidney disease (ADPKD), a common inherited kidney disorder. Although the channel is non-selective, Ca^{2+} can influence ion conduction at different concentrations[1] and cannot have outward permeation[2]. The detailed gating and activation mechanisms remain unclear, with two possible hypotheses: a π-to-α helix transition that leads to pore opening[1], or the π-helix bulge acting as a hinge[2]. In this work, we focus on explaining channel behaviour in the presence of Ca^{2+} and on the structural mechanisms that enable pore opening. Using molecular dynamics simulations, we systematically assess ion conduction rates under different ionic conditions, including K^+, Na^+ and Ca^{2+}, particularly when Ca^{2+} is present together with monovalent ions. Transitions between open and closed states are captured using enhanced sampling methods, and a dynamic model of the pore conformational landscape is constructed with Markov State Models (MSMs) to further explore the possibility of multiple gating and activation mechanisms. Our results provide a framework for understanding how TRPP proteins couple ion permeation, gating, and modulation factors, paving the way for future studies on TRPP channel modulation and ADPKD research.

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CAI - D3 - F05
The role of metal-ligand binding on natural product inhibitors of methyl-coenzyme M reductase

Anna Levison[1], Sokratis Stergiadis[1], Omar Cristobal-Carballo[2], Katerina Theodoridou[3], Mauricio Cafiero[1]
[1]University of Reading, UK; [2] Agri-Food and Biosciences Institute, UK; [3] Queen's University Belfast, UK

According to the 2022 IPCC report, agriculture contributes approximately 22% of net anthropogenic greenhouse gas emissions, with methane emissions from enteric fermentation in ruminant livestock representing a dominant source within the sector[1]. Given methane's global warming potential of roughly 28 times that of CO_2 over a 100-year time horizon, mitigation of enteric methane emissions represents a crucial target for tackling climate change[1]. Using methane-inhibiting additives that directly disrupt the ruminal methanogenesis pathway, with the key molecular target being methyl-coenzyme M reductase (MCR; the enzyme that catalyses the terminal step of methane formation)[2], can be fed to ruminants as a mitigation strategy. To evaluate candidate methane-inhibiting feed additives, the study employed in silico molecular docking using both traditional force-fields (FF) and a machine-learned interatomic potential (MLIP) to model protein-ligand interactions at the MCR active site. Using the FF-based docking framework focusing on the metal-ligand interactions, a panel of 24 plant-derived compounds, spanning a range of physicochemical properties and structural features, was evaluated. The docking identified methyl trans-geranyl acetate (-7.8 kcal/mol^{-1}), cinnamic acid (-7.4 kcal/mol^{-1}), and caffeic acid (-7.1 kcal/mol^{-1}) as the lowest-energy binding ligands, with predicted binding energies being consistently lower than those achieved using traditional docking methods (-7.4, -6.6, and -6.3 kcal/mol^{-1}, respectively). A set of benchmark compounds were also evaluated with the MLIP-based docking method for comparison to FF-based docking. These findings highlight some of the limitations of traditional docking scoring functions on overestimating the binding energies of some compounds and demonstrate MLIP-based docking as an improved tool for prioritising candidates for methanogenesis inhibition. MLIP-based docking can be recommended to support the shortlisting of plant-derived feed additives for further in vitro and in vivo evaluation of methane inhibitors for ruminants.

Financial support for this work has been provided by the Biotechnology and Biological Sciences Research Council (BBSRC) [grant number BB/T008776/1] as part of the Doctoral Training Partnership FoodBioSystems: biological processes across the Agri-Foodsystem from pre-farm to post-fork.

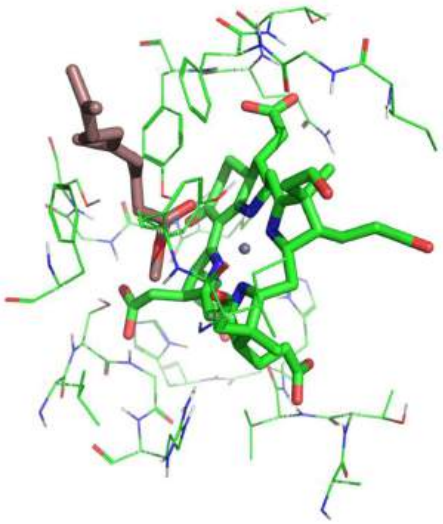

Figure 1: Methyl trans-geranyl acetate binding with Methyl-coenzyme M reductase (-7.8 kcal/mol^{-1})

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CAI - D4 - O01
The evolution of AI in scientific searching

Rosie Gibson[1]
[1]*CAS, A Division of the American Chemical Society, USA*

In the last two decades, the volume and complexity of scientific literature have surged in both quantity and complexity, driven by the rapid pace of discovery and the rise of interdisciplinary research. Navigating this expanding landscape and extracting meaningful insights has become increasingly time-consuming and requires significant scientific expertise. For years, CAS SciFinder® has been a trusted solution for scientists, providing expertly curated and indexed scientific information. The integration of science-smart AI into CAS SciFinder, with the largest human-curated collection of global scientific knowledge, provides faster, more relevant, and increasingly personalized results that continually improve with each search. Learn how these AI capabilities differ fundamentally from general AI tools, and how they can support your goals from accelerating research to supporting career advancement.

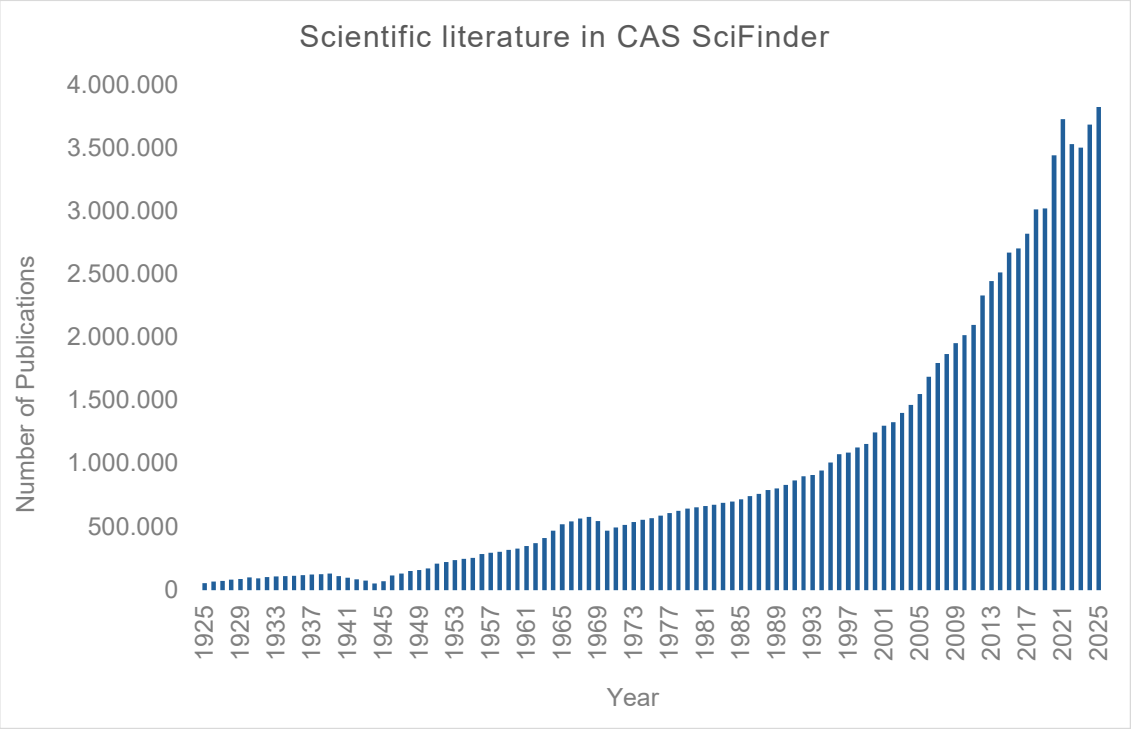

Fig. Number of publications from 1925-2025 in CAS SciFinder. Source: CAS Content Collection™.

CAI - D4 - O02

A machine-learning–driven multiscale investigation of low-cost thermochemical heat storage materials based on LiCl–LiBr solid solutions

Zhaochun Liu[1*],Veerapandian Ponnuchamy[1], Ionut Tranca[1], Frederik Tielens[1]
[1]*General Chemistry (ALGC), Materials Modelling Group, Vrije Universiteit Brussel (VUB), Belgium*

Thermochemical heat storage (TCHS) materials offer high energy density and long-term storage capability, but their large-scale deployment is presently limited by material cost, compositional instability, and poorly understood hydration mechanisms.[1-2] Alkali halide systems, such as LiCl–LiBr solid solutions, are promising low-cost and sustainable candidates due to their tunable thermodynamic properties and reversible hydration behaviour. However, rational material optimisation requires a systematic understanding of how anion substitution, atomic ordering, and hydration affect phase stability and structural response across compositions. In this work, we present a machine-learning–driven multiscale modelling framework to investigate LiCl–LiBr solid solutions as model TCHS materials. First-principles calculations reveal a pronounced asymmetry in anion substitution energetics: Br^- incorporation into LiCl stabilises the lattice through volumetric expansion and strain relief, whereas Cl^- substitution into LiBr induces lattice contraction and increased formation energies. At equimolar composition, different anion-distribution motifs with nearly identical lattice parameters exhibit substantial energetic differences, demonstrating that local configurational ordering—rather than bulk geometry—governs thermodynamic stability.

To access experimentally relevant length and time scales, machine-learning interatomic potentials were trained on first-principles data and applied in large-scale molecular dynamics simulations. These simulations confirm the structural robustness of mixed LiCl–LiBr phases, reproduce experimental lattice constants and densities with high fidelity, and accurately capture local coordination environments and radial distribution functions (Figure 1). Extensions to hydrated LiBr interfaces further demonstrate that the trained potentials reliably describe solid–water interactions, enabling future exploration of hydration-driven heat storage mechanisms.

Overall, this study establishes a systematic computational pathway for screening and understanding low-cost TCHS materials, highlighting the critical role of machine-learning potentials in bridging atomistic insight and materials design for sustainable thermal energy storage.

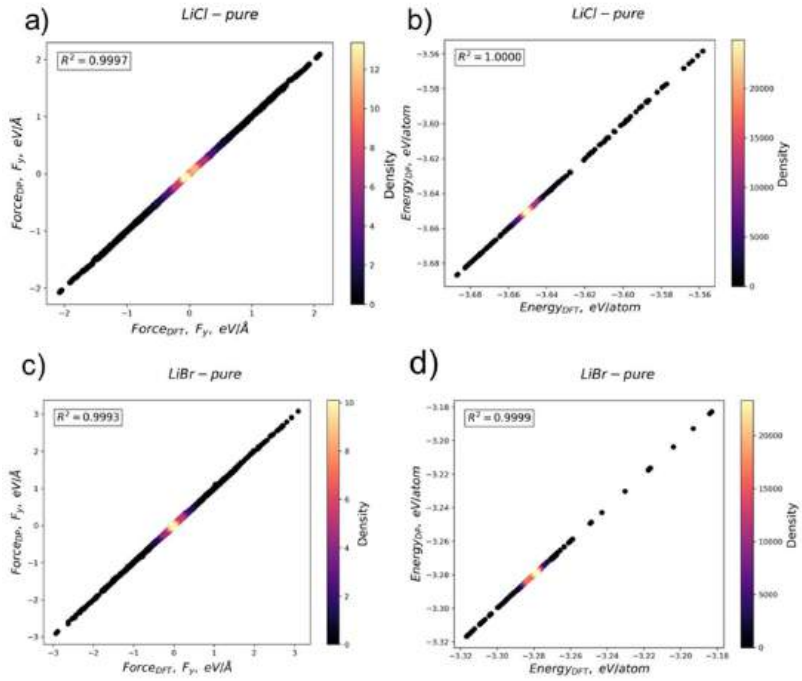

Fig.1. Correlation plots comparing DeepMD-predicted energies and forces with DFT reference values for (*a*–*b*) LiCl and (*c*–*d*) LiBr.

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CAI - D4 - O03
3D-QTAIM descriptor-based modeling for asymmetric catalysis

Mario Villares[1], Pau Morata[1], Maria Besora[1], Jorge J. Carbó[1]
[1]*Universitat Rovira i Virgili, Dept. de Química Física i Inorgànica, Spain*

In the fine chemicals and pharmaceutical industries, there is a great interest in developing highly efficient catalytic routes for obtaining complex, active molecules selectively. The computational prediction of catalytic outcome is very challenging, especially for enantioselectivity because the energy differences responsible for enantiomeric enrichment can be as low as 1-3 kcal·mol^{-1}. Recently, the use of statistical Machine Learning techniques has emerged as a new paradigm in computational catalysis. Studies in this area relay in chiral-type, molecular descriptors derived from 3D structures.
Here, we will present our work aiming to construct regression models able to predict asymmetric organometallic catalysts using our newly developed 3D-QTAIM descriptors, which relay on properties derived from *Quantum Theory Atoms in Molecules* (QTAIM), and on alignment-independent transition metal-centre correlograms and graph representation of molecular systems. The automatic generation of descriptors and regression models (over 1 million for each dataset) allows to optimize the QTAIM properties and vectorization parameters. Depending of the data regime the models are built with Partial
Least Squares (PLS) and Graph Neural Networks (GNN) algorithms. At low data regime, we improve the statistical parameters of previous models developed in our laboratory: asymmetric hydroformylation by Rh-diphosphine using QM-GRIND descriptors[1] and asymmetric cyclopropanation by Cu complex using MolQuO descriptors.[2] Descriptors capture the stereoelectronic properties of the catalysts and predict both enantioselectivity and activity. At large data regime, 3D-QTAIM descriptors build regression models for Vaska's complex data set,[3] indicating their universal character.

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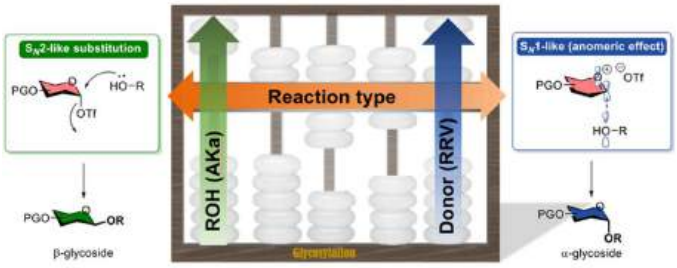
CAI - D4 - O04
AI and statistical analysis for understanding stereoselective glycosylation reactions

Cheng-Chung Wang[1]
[1]*Institute of Chemistry, Academia Sinica, Taiwan*

Carbohydrates are ubiquitous biomolecules that mediate numerous biological processes and exhibit important pathogenic effects. However, chemical synthesis of glycoconjugates has been hampered by challenges in glycosylation reaction, of which the stereoselectivity and yield are paramount but unpredictable. We develop a database composed of relative reactivity value (RRV) [1,2] and acceptor nucleophilic constant (Aka)[3] to quantify the reactivity of glycosyl donors and nucleophilicity of hydroxyl groups in glycosylation influenced by the steric, electronic and structural effects, providing a connection between experiments and computer algorithm. A diverse range of glycosylation donors and acceptors with well-defined reactivity and promotors were organized and processed by the designed program “GlycoComputer” for prediction of glycosylation reaction without involving sophisticated computational processing. The applicability of this system was further tested by the synthesis of a Lewis A skeleton to show that the stereoselectivity and yield can be accurately estimated.[4]



A glycocomputer-based framework for predicting stereoselective outcomes in glycosylation reactions based on reaction type, donor reactivity (RRV), and acceptor nucleophilicity (Aka).

We thank National Science and Technology Council (NSTC), Taiwan and Academia Sinica, Taiwan for their financial support for these works.

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CAI - D4 - O06
Water and CO desorption from amorphous carbon surfaces: A computational and experimental study

T. Vorsselmans[1], E. C. Neyts[1], I. Grubova[1], T. Suhasaria[2], V. Leuschner[2,3], C. Jäger[2], Th. Henning[2]
[1]Research Group MOSAIC, Dept. of Chemistry, University of Antwerp, Belgium; [2]Max Planck Institute für Astronomie, Germany; [3]Dept. for Physics and Astronomy, University of Heidelberg, Germany

Carbon dust is a major dust component. The desorption study of volatile molecules on carbonaceous interstellar dust is crucial for understanding the chemistry and physics of dense clouds and protoplanetary disks, providing insights into star and planet formation. In this work, laboratory findings are complemented by computational studies. Experimentally, carbon dust analogs were produced via laser ablation of graphite and condensed onto gold surfaces. We explored the interactions of the two most abundant ice components, water and carbon monoxide, using temperature-programmed desorption (TPD) and reflection-absorption infrared spectroscopy (RAIRS). Desorption behaviour from sub-monolayer and monolayer coverages indicate different binding sites across the surface resulting in distinct desorption peaks and higher desorption energies than those reported in the literature for HOPG and amorphous solid water surfaces. Computationally, both quantum mechanical calculations at the DFT/PBE0/D3 level as well as classical enhanced sampling calculations were carried out. The DFT results yield ranges of binding energies that are consistent with the experimental results and provide insight into how bent and/or defective graphene sheets affect the binding energies. The classical simulations consist of well-tempered metadynamics using the flexible spc/Fw model for water and a dedicated Lennard-Jones potential for water/graphene interactions. These calculations yield free energy profiles for desorption. Based on these data, simulated TPD spectra can be calculated that are in fair agreement with the experimental spectra. This combination of both experimental and computational techniques yields a multifacetted view on the desorption of astrochemically highly relevant molecules from dust particles.

CAI - D4 - O07

Multi-scale investigation of triboelectric nanogenerator: An expanded DFT calculation based on machine learning

Yongsheng Huang[1], Mitsuhiro Matsumoto[1]
[1]Kyoto Univ., Dept. of Mechanical Engineering and Science, Thermal Science and Engineering Laboratory, Japan

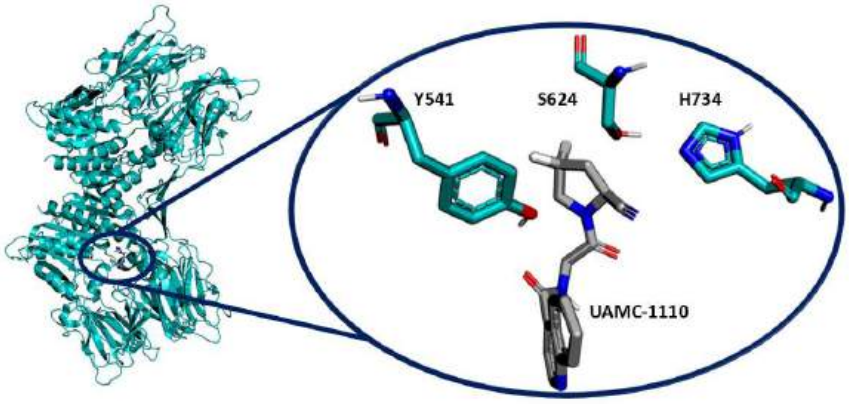
Triboelectric nanogenerators (TENGs) operate through coupled electron transfer, ion migration, and mechanochemical effects; however, the disparate spatial and temporal scales of these processes hinder a quantitative understanding of their individual contributions. In this work, we investigate nanoscale electron transfer mechanisms using density functional theory (DFT) calculations for two representative insulating polymers, polyvinyl chloride (PVC) and polyvinyl alcohol (PVA). Based on the DFT-derived electronic information, machine learning interatomic potentials are constructed using the DeepMD-kit, enabling large-scale molecular dynamics simulations within the LAMMPS framework.

The simulations reveal that electron transfer plays a primary role in establishing the triboelectric potential difference, whereas subsequent ion migration partially compensates the accumulated charge, leading to a reduction in the effective power output. This study establishes a multi-scale simulation framework that bridges quantum-level charge transfer with mesoscale dynamics, offering mechanistic insight into competing charge transport processes and providing guidance for the rational design of high-performance TENG materials.

CAI - D4 - O08
Binding mechanism of UAMC-1110 to fibroblast activation protein

Joep W. Wals[1], Rui P. P. Neves[2], Pedro A. Fernandes[2], Hans De Winter[1]
[1]Laboratory of Medicinal Chemistry, Dept. of Pharmaceutical Sciences, University of Antwerp, Belgium; [2]LAQV@REQUIMTE, Dept. de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Portugal

Fibroblast activation protein (FAP) is an enzyme highly expressed in cancer-associated fibroblasts (CAFs)[1]. Over the past years, several FAP inhibitors (FAPIs) have been developed for tumor diagnosis[2]. In these strategies, a chelator is attached to a small molecule binding to FAP. Longer tumor retention times for FAPIs are desirable to enable a theranostic approach, which combines diagnosis and therapy. Therefore, we aimed to elucidate the binding mechanism of our in-house designed FAPI frontrunner, UAMC-1110[3]. Initial molecular dynamics simulations of the ligand led to a non-covalent starting structure. Subsequent QM/MM calculations were performed to investigate the covalent binding mechanism of UAMC-1110. This study shows that the compound initially forms a covalent complex with the receptor after a proton transfer from S624 to H734 and a concerted, asynchronous nucleophilic attack of S624 on the nitrile warhead. The resulting imidate anion can be stabilized via two routes: 1) protonation via H734 through two water molecules; 2) direct protonation by Y541 followed by protonation restoration. Additional covalent MD simulations on the intermediate and product complex showed that direct protonation of the imidate anion by either H734 or Y541 is plausible. These results highlight that UAMC-1110 binds reversibly to FAP and shows the potential for other ligands to form an irreversible covalent complex to increase tumor retention times.



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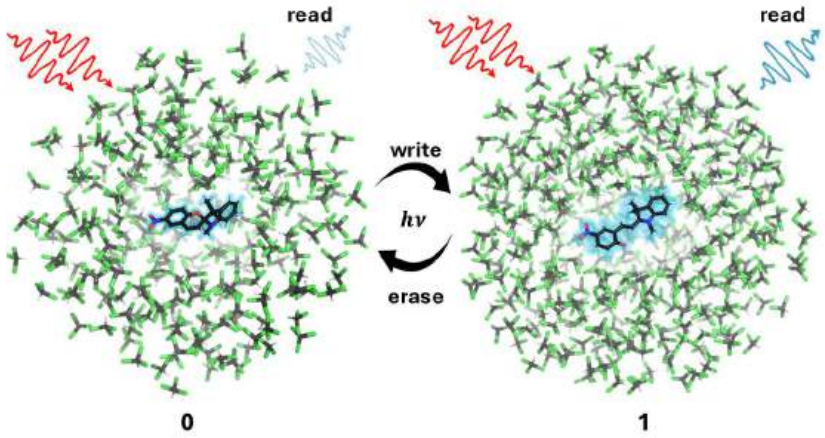
CAI - D4 - O09

Realistic simulations of nonlinear optical photoswitches with novel all-atom quantum mechanical methodologies

Marilù G. Maraldi[1], Vincent Rodriguez[2], Frédéric Castet[2], Marc de Wergifosse[1]
[1]IMCN, UCLouvain, Belgium; [2]ISM, University of Bordeaux, France

Molecular photoswitches can serve as nanoscopic switching elements in photonic and electronic devices. One appealing application is the use of such systems as optical memories. For this purpose, one must be able to read the state of the photoswitch either closed form (bit = 0) or open form (bit = 1) without inducing the photoswitching. A solution for reading the state of the switch is to exploit nonlinear scattering effects, such as the second-harmonic generation (SHG), that allows to distinguish photoisomers without triggering linear absorption photoswitching. Designing efficient photoswitches with enhanced SHG contrast remains a challenge. Theoretical chemistry plays a crucial role in understanding and guiding such molecular design[1,2].
A predictive theoretical and computational protocol should be able to capture the complexity inherent to experiments. This should include explicit solvent and dynamic-structural effects in an all-atom quantum mechanical (AQM) approach to compute SHG and UV-Vis absoprtion[2]. Traditional QM methods face a computational wall when dealing with large and realistic systems. In the last decade, simplified quantum chemistry methods (sQC) have enabled AQM-level simulations for large systems[3] (thousands of atoms). Recently, de Wergifosse[4] introduced the eXact integral simplified time-dependent density functional theory (XsTD-DFT). With a significant lower cost, recent works[4-6] demonstrate that XsTD-DFT is as reliable and robust as conventional TD-DFT methods to compute optical properties.
In this work, we present an AQM protocol that combines molecular dynamics at the semi-empirical level with XsTD-DFT to compute the SHG of spiropyran/merocyanine photoswitches explicitly accounting for the solvent. Results are in striking agreement with respect to experiments.
This methodology provides a powerful framework for the predictive design of next-generation NLO molecular photoswitchable materials, offering complementary insights into the interplay between dynamic-structural and environment effects. While the ADQM methodology allows to treat the interactions at the QM level, the computational cost remains reasonable.



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CAI - D4 - O10
Asymmetrically-constrained adiabatic ALMO-EDA: Designing catalysts from first principles

Markus G. S. Weiss[1,2], Alistair J. Sterling[1]
[1]The University of Texas at Dallas, USA; [2]RWTH Aachen University, Germany

Intermolecular interactions are integral to the efficiency and selectivity of catalytic processes. Even subtle stabilization of transition states (TS) by such interactions can lead to significant enhancements in reaction rates, underscoring the importance of understanding the underlying relationships between interaction and activity. Traditional energy decomposition analysis (EDA) methods, including the absolutely localized molecular orbital EDA (ALMO-EDA), offer valuable insights into the nature of ground state interactions, such as electrostatics, Pauli repulsion, dispersion, polarization, and charge transfer. However, while isolating the contributions of individual interactions to catalysis remains a challenge, it is essential for the rational design of efficient catalysts.
In this work, we introduce an asymmetric adiabatic ALMO-EDA framework to switch on individual interactions between the catalyst and the TS structure, providing a direct causal link between catalyst structure and activity. We apply this methodology to pericyclic and nucleophilic addition reactions, to dissect the specific roles of each interaction component. Our findings reveal distinct classes of catalysts that lower activation barriers through common mechanisms, such as strong electrostatic interactions, significant polarization effects, and charge transfer mechanisms. By systematically analyzing these contributions, we offer actionable insights for the rational design of both organocatalysts and Lewis acid catalysts.
By uncovering how specific intermolecular interactions contribute to catalysis, our approach establishes a generalizable framework for studying a wide array of catalytic systems. Our ongoing research aims to extend this methodology to more complex catalytic processes, advancing the field of catalyst design by predicting the impact of individual intermolecular interactions on reaction kinetics.

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CAI - D4 - O11
All correlation within a mean field: Assessment of i-DMFT and the modified Collins conjecture

Florian Matz[1,2], Paul Graf[1,2], Markus Penz[1,2], Christian Schilling[1,2]
[1]Faculty of Physics, Arnold Sommerfeld Centre for Theoretical Physics (ASC), Ludwig Maximilian University Munich, Germany; [2]Munich Center for Quantum Science and Technology (MCQST), Germany

Despite decades of development, there are still few computational methods that achieve a holistic description of electron correlation, so that calculations routinely neglect significant parts of the energy. In this work, we assess how a variation of one-particle reduced density matrix functional theory (RDMFT)[1], dubbed information-(i-) DMFT[2], can recover the accuracy of configuration interaction methods including all correlation with a cost comparable to Hartree-Fock.
i-DMFT is based on the modified Collins conjecture[3] that relates the entropy of the one-particle density matrix with the correlation energy and highlights the possible synergies between quantum information theory and quantum chemistry.[4]
We critically investigate the validity of this conjecture for examples from simple model systems over diatomics to larger molecules. While charge localisation and bond compression can lead to deviations, the conjecture holds for molecular deformations, bond dissociation, and even chemical reactions and is generalisable for chemically similar molecules. We also present the first-time investigation of Collins' conjecture for excited states. Finally, we apply i-DMFT to obtain dissociation curves and reaction profiles with near-FCI accuracy and analyse the accuracy of one-particle observables.
The work contributes to a paradigm shift in computational chemistry that involves a maximally efficient representation of many-body complexity, made possible by interdisciplinary efforts of theoretical physicists and computational chemists. Motivated by this, we also compare it to similar modern methods such as QICAS[5] and wave function interpolation[6].

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CAI - D4 - F01

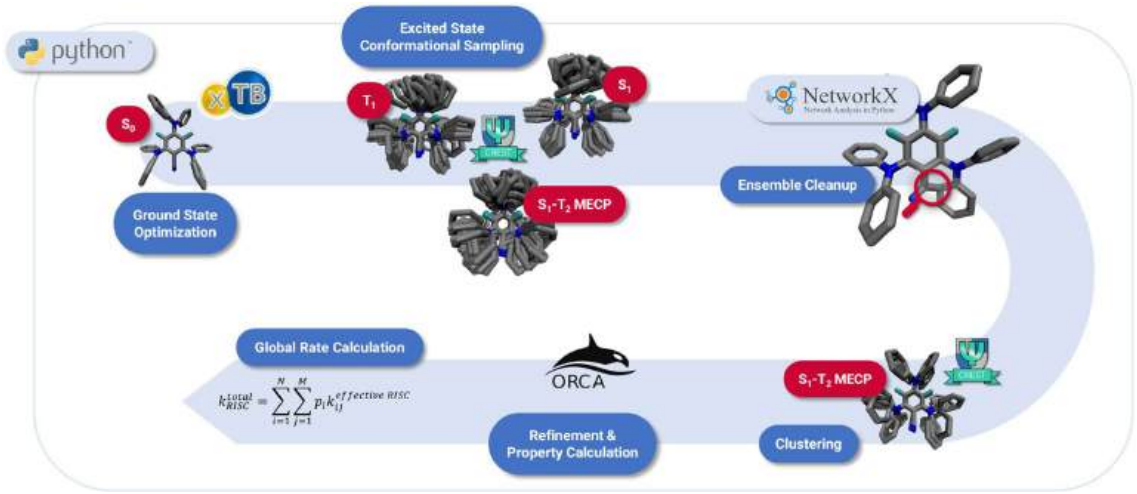
Towards automated ensemble-averaged kinetics of reverse intersystem crossing in flexible TADF emitters

Jonas Weiser[1], Christian Wiebeler[1]
[1]*Institute of Physics, University of Augsburg, Germany*

Thermally activated delayed fluorescence (TADF) is a cornerstone of third generation OLED design, enabling up to 100% internal quantum efficiency through reverse intersystem crossing (RISC).[1] However, in flexible donor-acceptor systems, RISC rates are sensitive to geometry-dependent fluctuations in energy gaps and spin-orbit couplings (SOCs).[2] Traditional static models relying on single optimized geometries often fail to capture the experimental reality of these flexible molecules, as they not only ignore the distribution of accessible excited-state conformations but also RISC pathways governed by higher-order spin-vibronic coupling via intermediate higher triplet states[3].

To address this, we present an automated quantum-chemical workflow that moves beyond static geometry approximations and bridges the gap between microscopic structural dynamics and macroscopic kinetic rates. The pipeline integrates large-scale metadynamics sampling[4] of S_1 and T_1 states as well as S_1–T_2 crossings[5] with structural clustering to identify key representative macrostates. We then employ efficient electronic structure theory[6] to refine geometries, energies, and SOC matrix elements across the resulting conformational space.

Integrating these local contributions, our approach calculates a global RISC rate as a Boltzmann-weighted sum of all local direct and T_2-mediated pathways. This framework accurately captures molecular flexibility and provides a physically rigorous and scalable tool for the reliable prediction of TADF RISC rates across a diverse chemical space.



Scheme illustrating the individual workflow steps.

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CAI - D4 - F02

From nature's layers to neural layers: An AI and machine learning approach to tomato preservation via an edible pseudoprotein coating

Ilona Shekiladze[1], Salome Cheishvili[2], Tamar Phalavandishvili[3], Ramaz Katsarava[4]
[1]Bachelor's Student, Chemical and Biological Engineering, GTU, Georgia; [2]Phd Student, Chemical and Biological Engineering, GTU, Georgia; [3]Associate Professor, Department of Chemical and Biological Technologies, GTU, Georgia; [4]Professor, Director of the Institute of Chemistry and Molecular Sciences, Agricultural University, Georgia

Modern food storage increasingly focuses on environmentally friendly and biodegradable technologies. Tomatoes (*Lycopersicum esculentum*), as highly perishable vegetables, require innovative storage methods. This study investigates the effectiveness of pseudoprotein food coatings during tomato storage and models the process dynamics using classical mathematical methods and AI.

The coating, synthesized from natural α-amino acids, was applied to tomato samples at two different thicknesses controlled by immersion times of 10s and 30s. Samples were stored under two temperature regimes (10–12°C and 20–22°C) for 13-45 days. A full factorial experimental design (2^3) was used to study tomato storage. A linear regression equation was obtained using the matrix method, with soluble dry matter (Brix°) as the optimization parameter. In parallel, symbolic regression using PySR (Symbolic Regression in Python) was applied to develop a mathematical model describing the dynamics of soluble dry matter. Machine learning algorithms were also used to predict weight loss trends, allowing reliable prediction of weight loss in pseudoprotein-coated tomatoes up to 45-55 days.

Overall, the study demonstrates that coating properties and storage temperature significantly influence tomato quality, while pseudoprotein coatings partially reduce the negative effects of higher temperatures.

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CAI - D4 - F03

Theoretical study of collision induced dissociation mechanism for PO3G 77-59 m/z ion: When MS2 energy data and quantum chemistry reveals hidden molecular structuresd

Vinicius Kuchenbecker[1], Nelson H. Morgon[1]
[1]UNICAMP, Brazil

In Energy-Resolved Tandem Mass Spectrometry (ERMS), ion intensities are recorded as a function of collision acceleration energy. When combined with theoretical modeling, ERMS enables mechanistic interpretation of fragmentation pathways.[1] However, such correlations remain scarce, and none have been reported for the poly(trimethylene ether) glycol (PO3G) dimer. Establishing this relationship is essential for understanding the physical chemistry of its gas-phase dissociation.[2] A principal dissociation pathway of the PO3G dimer was investigated by integrating ERMS experiments with quantum-chemical calculations based on transition state theory (TST) and CCSD(T)/CBS electronic structure methods. Mass spectra acquired using an Orbitrap Exploris 120 revealed characteristic fragmentation leading to the 77 and 59 m/z ions. Survival-yield analysis supports the proposal that ion 77 m/z acts as the primary precursor of 59 m/z. Constitutional isomer enumeration using ForMileS[3] showed that both fragments correspond to a single significantly more stable structure relative to alternative isomers. Reaction pathways connecting 77 to 59 m/z were mapped using DFT-optimized geometries followed by CCSD(T)/CBS single-point refinements. Benchmarking indicated that PBE0/def2-TZVP best reproduced CCSD(T)/CBS barrier heights, while PBE0/aug-cc-pVQZ was employed for frequency calculations. Comparison of computed barriers with ERMS profiles indicates that, due to limited internal energy in secondary fragments, the lower-barrier pathway yielding a protonated allylic alcohol is kinetically favored, although an alternative oxonium structure is thermodynamically more stable. This combined ERMS–TST approach provides mechanistic insight into PO3G fragmentation and establishes a framework for interpreting MS2 pathways of small oligomers.

Acknowledgements to UNICAMP Institute of Chemistry and Chemyunion LTDA.

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Chemistry Meets Biology & Food Science (CBF)

CBF - D1 - O01

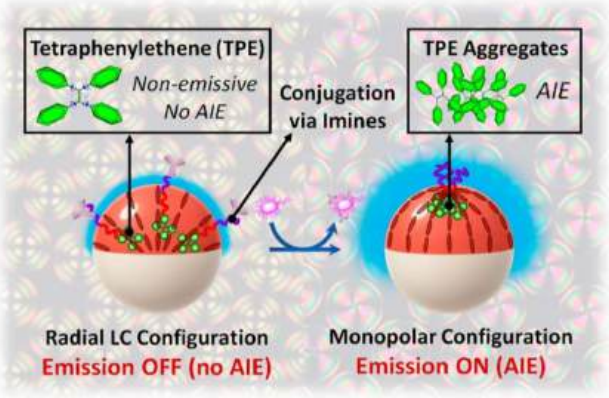
Dynamic complex liquid crystal emulsions as responsive optical platforms for detecting foodborne pathogens

Mauricio Vera-Arévalo, Alberto Concellón
Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain.

Liquid crystals (LCs) are dynamic soft materials that combine long-range order with fluidity, enabling applications in optics, sensing, and soft robotics.[1] When confined within micrometer-sized emulsion droplets, LCs adopt distinct internal organizations that are highly responsive to molecular-level perturbations occurring at the LC/water interface.[2] LC emulsions are therefore promising platforms for sensing technologies in which LC alignment acts as an amplifier of local interfacial events, resulting in pronounced optical appearance changes.[3,4] However, most LC-based sensors rely on polarized-light optical microscopy, which limits quantitative analysis and practical deployment.

Here, we report a fluorescence-based transduction scheme that converts LC ordering transitions into quantitative optical outputs. Our strategy employs amphiphilic block copolymers bearing aggregation-induced emission (AIE) motifs that undergo dynamic covalent conjugation with IgG antibodies through reversible imine chemistry. In complex LC emulsions, the polymer surfactants localize differently depending on the droplet LC configuration: accumulation at monopolar defects concentrates AIE units to generate a bright ON state, whereas redistribution along the LC/W interface in the radial configuration suppresses emission, yielding an OFF state. Recognition of foodborne pathogens (e.g., *Salmonella* or *Listeria*) reversibly perturbs this equilibrium, producing rapid (~1 h) ON/OFF fluorescence responses with detection limits down to 10^2 cells/mL. These detection limits are competitive with state-of-the-art biosensing approaches while avoiding enrichment steps or specialized instrumentation, enabling quantitative readouts using simple and potentially portable fluorimeters. Incorporation of a ratiometric reference dye further enhances robustness against experimental variability, relaxing requirements on droplet monodispersity or microfluidic fabrication and enabling reliable measurements.

Overall, this work establishes fluorescence transduction of LC ordering transitions as a generalizable and practical sensing paradigm, bridging soft matter design with real-world diagnostics.



This work was financially supported by the projects PID2023-146811NA-I00 and RYC2021-031154-I, funded by MICIU/AEI/10.13039/501100011033 and “ERDF A way of mak-ing Europe”; and Gobierno de Aragón–FSE (research group E47_23R). MVA thanks MICIU/AEI for his PhD grant (FPU24/01406).

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CBF - D1 - O02

Development of a molecular beacon-based LAMP assay for the specific identification of *Ginkgo biloba* in commercial herbal products and food supplements

Vânia Rodrigues[1], M. Alice Pinto[1], Joana S. Amaral[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal

Ginkgo biloba is widely used in herbal products and plant food supplements (PFS), but its high demand and market value increase the risk of botanical adulteration, underscoring the need for accurate detection methods to safeguard authenticity and consumer safety[1]. Although DNA-based methods are the most suited for detecting species substitutions, DNA recovery from processed PFS is often compromised by pharmaceutical excipients that hinder DNA extraction[2]. Moreover, rapid and simple approaches for on-site screening (e.g., verification of powdered ingredients, inspections, border control) are of particular interest for prioritizing potentially adulterated samples for subsequent laboratory confirmation. In this context, loop-mediated isothermal amplification (LAMP) is particularly suitable, as it enables rapid, highly specific DNA amplification at constant temperature with minimal instrumentation, supporting on-site screening[3].

In this work, a colorimetric LAMP assay targeting the ITS1 region was first proposed for the specific detection of *G. biloba* using a five-primer set. *In silico* analysis supported the assay specificity, but only one loop primer could be designed. Because false positives occurred in the no-template control (1/10), the assay was modified to incorporate a molecular beacon (MB-LAMP) to enhance specificity. Fluorescence MB-LAMP enabled detection at 65 °C within 30 min, eliminated false-positive signals, and showed high specificity, discriminating *G. biloba* from the adulterant *Sophora japonica* and 49 additional medicinal plant species. High sensitivity was achieved, with a limit of detection of 1 pg *G. biloba* DNA. The method was applied to 11 commercial infusions, detecting *G. biloba* in all samples. Additionally, given the complexity of PFS matrices, five DNA extraction procedures were compared using real-time PCR and MB-LAMP. NucleoSpin® Soil produced the highest positivity by real-time PCR (9/14), whereas NucleoSpin® Plant II performed best with MB-LAMP (4/14). Although real-time PCR was more sensitive overall, MB-LAMP provides a faster and operationally simpler workflow suitable for first-line, on-site screening.

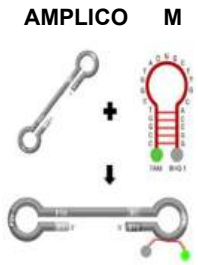

Fig. 1. Schematic representation of the molecular beacon (MB) and its hybridization to the target amplicon for fluorescence reading.

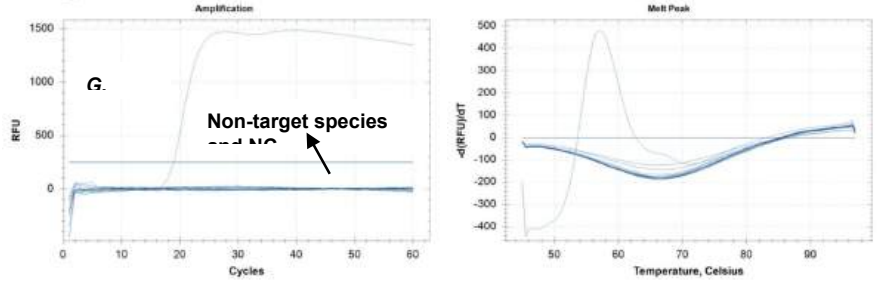

Fig. 2. Evaluation of MB-LAMP specificity for the authentication of *G. biloba* using DNA extracts from 50 medicinal plants; fluorescence amplification (left) and melting analysis (right).

Acknowledgements: To the Foundation for Science and Technology (FCT, Portugal) for financial support of the project "POIROT: novel methods and approaches for detecting the illegal addition of Pharmaceutical drugs and bOtanIcal adulteRatiOn in plant food supplements" (DOI: 10.54499/PTDC/SAU-PUB/3803/2021). This work was also supported by national funds through FCT/MCTES (PIDDAC): CIMO, UIDB/00690/2020 (DOI: 10.54499/UIDB/00690/2020) and UIDP/00690/2020 (DOI:10.54499/UIDP/00690/2020); and SusTEC, LA/P/0007/2020 (DOI:10.54499/LA/P/0007/2020).

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CBF - D1 - O03
Fluorescent sensor array for fungal detection and VOC-based quality monitoring in citrus fruit

Alessia Cavallaro[1], Rossella Santonocito[1], Federico La Spada[2], Rossana Parlascino[2], Mario Riolo[2], Santa Olga Cacciola[2], Nunzio Tuccitto[1], Giuseppe Trusso Sfrazzetto[1]
[1]Dept. of Chemistry, University of Catania, Italy; [2]Dept. of Agriculture, Food and Environment, University of Catania, Italy

The early detection of plant pathogenic fungi, as well as the assessment of conservation status in citrus fruit, is crucial for ensuring food safety and protecting human health. Here, we present a supramolecular fluorescent sensor array as a versatile platform for the monitoring of fungal contamination and quality status of citrus fruit. The array consists of multiple organic fluorescent probes with different recognition sites, enabling interactions with a broad range of analytes through non-covalent forces (hydrogen bonding, π-π stacking, ion-dipole). This approach generates characteristic fluorescence response patterns that act as optical fingerprints, enabling the discrimination of complex food samples.[1] First, we demonstrate the instant identification of pathogenic fungi from citrus washing waters, before the appearance of visible symptoms.[2] The system is interfaced with a smartphone, offering a easy-to-use detection tool for on-site monitoring. Secondly, the sensor array allows the non-invasive monitoring of packaged citrus fruit by analyzing volatile organic compounds (VOCs) emitted during ripening and fungal infection,[3] using an optical fiber-based detection setup.[4] The supramolecular nature of the array enables the simultaneous recognition of multiple VOCs, providing a comprehensive view of the fruit's metabolic and pathological state.
These results demonstrate the fluorescent sensor array as a sensitive, versatile, and portable tool for food quality control, representing a step toward next-generation agri-food monitoring technologies.

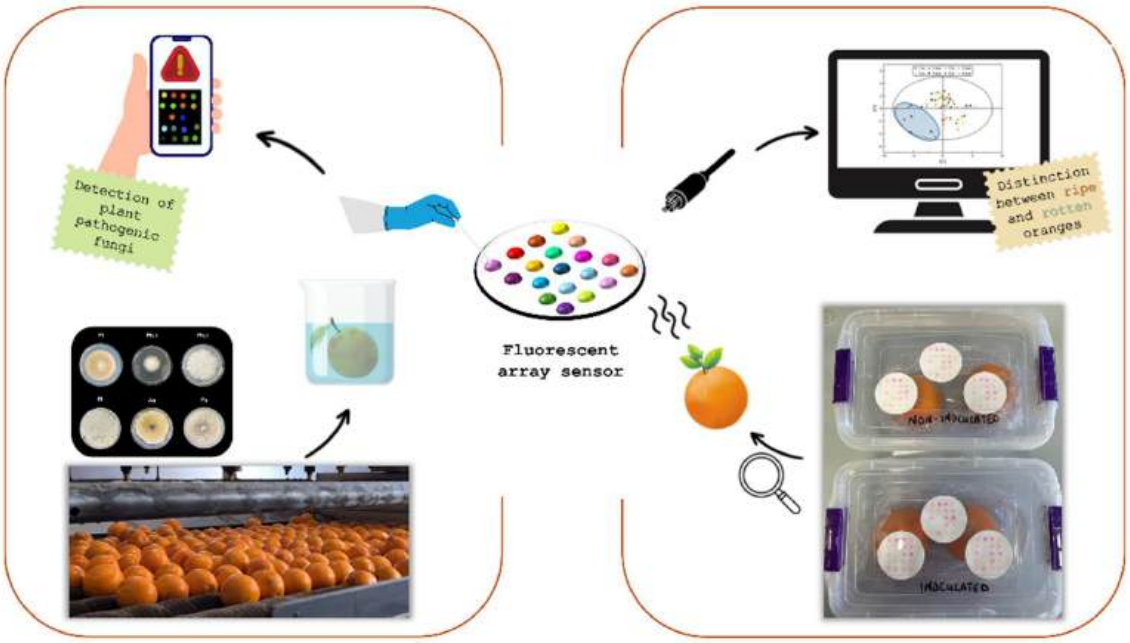

Fig. 1. Fluorescent sensor array for the detection of plant pathogenic fungi and citrus' VOCs.

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CBF - D1 - O04

Evaluation of functionality and migration behavior of nano Ag/PHBHHx films for packaging applications

Dries Hermans[1,*], Andrej Andjelic[1], Chris Vanheusden[1], Pieter Samyn[2], Hans Steenackers[3], Wim Deferme[4], Anitha Ethirajan[5], Jan D'Haen[6], Wouter Marchal[7], Mieke Buntinx[1]

[1]University of Hasselt, Materials and Packaging Research & Services, Belgium; [2]Sirris, Belgium; [3]KU Leuven, Centre of Microbial and Plant Genetics, Belgium; [4]University of Hasselt, Functional Materials Engineering, Belgium; [5]University of Hasselt, Nanobiophysics and Soft Matter Interfaces, Belgium; [6]University of Hasselt, Analytical & Microscopical Services, Belgium; [7]University of Hasselt, Analytical & Circular Chemistry, Belgium

Silver nanoparticles (Ag NPs) have been widely studied for incorporation in polymers to develop active packaging. This concept shows promise for improving the application potential of biopolymers such as poly(3-hydroxybutyrate-co-3-hydroxyhexanoate (PHBHHx). However, the functionality and migration behavior are highly dependent on the size, distribution, and surface-availability of the Ag NPs. Therefore, this study systematically compares the optical, oxygen barrier, and antimicrobial properties and migration mechanisms between Ag/PHBHHx films with Ag NPs distributed in the bulk and deposited at the surface.

Commercial spherical Ag NPs (50 nm, ± PVP-coating) were incorporated into PHBHHx films via two methods: bulk-mixing (extrusion and compression molding; 0.2 and 2.0 wt.%) and surface-coating (ultrasonic spraying of encapsulated NPs (10 and 40 wt.%, 50 layers). Optical properties (color, opacity, UV-VIS transmittance), Ag content, NP dispersity, oxygen permeability, and antimicrobial activity (*S. Aureus*, *E. coli*) were characterized. Migration (Ag°/Ag+) was quantified via SP-ICP-MS over 10 days at 40°C in food simulants A and B (EU 10/2011).

While bulk-mixing (0.2, 2.0 wt.% Ag) notably changed optical properties and improved oxygen barrier performance of the films, surface-coating (0.0014, 0.0060 wt.% Ag) had less impact on color, opacity, and no improvement in oxygen permeability, attributed to the different Ag NP distribution and silver content. Surface-coated films demonstrated superior antimicrobial efficacy (complete inactivation) compared to bulk-mixed films, due to the increased surface availability of Ag NPs. SP-ICP-MS analysis linked this to rapid desorption and continuous dissolution kinetics, contrasting with the slow diffusion observed in bulk-mixed samples. While migration levels in food simulant A remained below the regulatory limit (< 50 µg/kg), the surface-coated samples were non-compliant (> 50 µg/kg) in acidic food simulant B.

Overall, this study highlights the impact of Ag NP distribution and surface-availability on film functionality and migration, which is crucial for the development of safe active packaging materials.

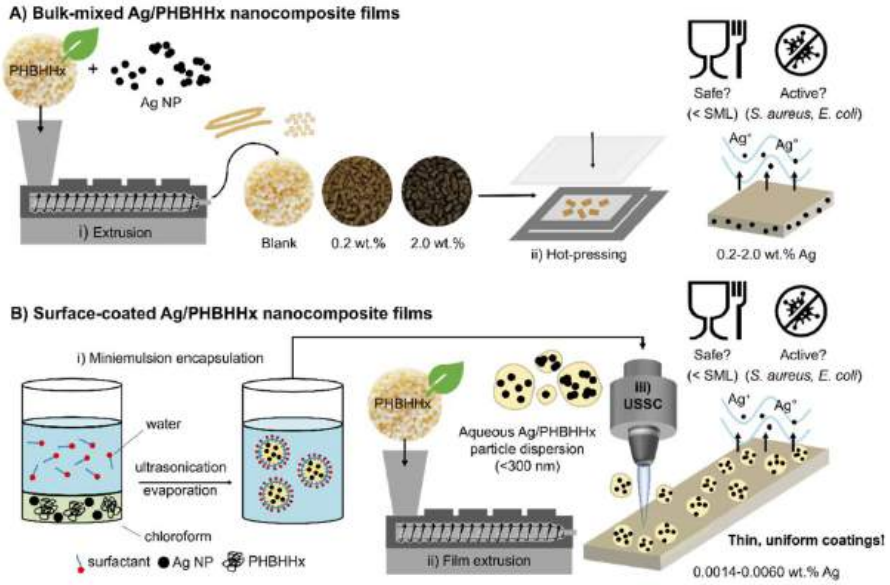

Fig. 1. Schematic overview of Ag/PHBHHx nanocomposite films processed via bulk-mixed (A) and Surface-coated (B) approach.

CBF - D1 - O05

Development of a real-time PCR assay for the detection of *Bombyx mori* (silkworm) in insect-based food and feed products

Vânia Rodrigues[1], M. Alice Pinto[1], Maria Villa[1], Joana S. Amaral[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal

Bombyx mori (silkworm) is a protein-rich insect authorised in the EU as a feed ingredient but not for human consumption[1]. Its extensive use in silk production generates large amounts of protein-rich by-products[2]. As the commercialization of insect-based foods grows, these by-products may enter different supply chains, increasing the risk of adulteration. Ensuring product authenticity is therefore essential to prevent food fraud and safeguard quality. In this context, the development of sensitive and specific molecular methods is essential for accurately identifying *B. mori* in food and feed products[3]. In this study, a real-time PCR (qPCR) assay targeting the sex-specific storage protein 1 (SP1) gene of *B. mori* (GenBank: EU273729.1) was developed. For that purpose, new primers and TaqMan probe were designed. Primers and probe specificity were validated using DNA from 74 different species, including insects (n=27), worldwide edible insects (n=25), cereals/seeds/legumes (n=7), spices/herbs (n=8) and seafood (n=7). No cross-reactivity was observed with non-target species, confirming the high specificity of the assay. qPCR parameters of efficiency, slope and R^2 were all within the acceptance criteria (Fig.1). To assess the quantitative performance, binary mixtures of powdered *B. mori* in *Acheta domesticus* (cricket) flour were prepared at known proportions (50%, 30%, 20%, 10%, 5%, and 1%). Mixtures with 25%, 15%, 7.5%, and 2.5% were used for validation purposes. A calibration curve enabled the accurate estimation of *B. mori* content in the validation mixtures, with errors between −13.62% and 5.87%, and coefficients of variation between 0.14% and 0.63%. An additional calibration curve was generated using commercial poultry feed, showing similar efficiency for *B. mori* detection. The assay was further applied to 30 commercial food and feed products labeled as containing insects.
Overall, the developed qPCR assay demonstrated high selectivity and sensitivity, enabling quantitative estimation and effective detection of *B. mori* in complex matrices.

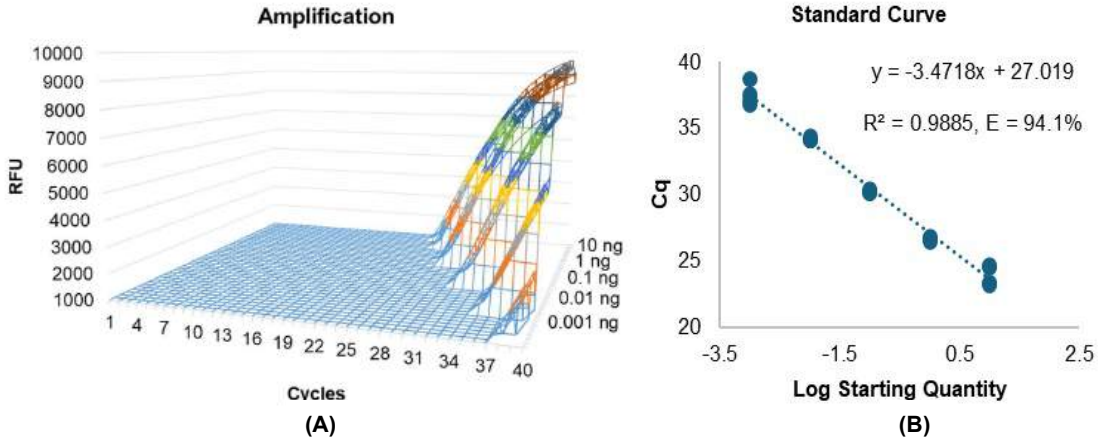

Fig. 1. Amplification curves (A) and calibration curve (B) of qPCR targeting the SP1 gene of *B. mori*. The amplified extracts correspond to 10-fold serially diluted *B. mori* DNA ranging from 10 ng to 0.001 ng (n=8 replicates).

Acknowledgements: To the Foundation for Science and Technology (FCT, Portugal) for financial support of the project "INSECTRAK - Advanced methods for the rapid detection of fraudulent insect addition in food and the authentication of insect-based novel food (2023.15568.PEX). This work was also supported by national funds through FCT/MCTES (PIDDAC): CIMO, UIDB/00690/2020 (DOI: 10.54499/UIDB/00690/2020) and UIDP/00690/2020 (DOI:10.54499/UIDP/00690/2020); and SusTEC, LA/P/0007/2020 (DOI:10.54499/LA/P/0007/2020).

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CBF - D1 - O06

Fermentation-induced molecular remodeling in South African indigenous tubers: Cassava and cocoyam

Alejandro Mendoza Cantu[1], Motseoa Lephatsi[2], Yusuf Abass[2], Ndiko Ludidi[3], Peter Bamidele[4], Fidele Tugizimana[2], Julia M. Gauglitz[1], Wout Bittremieux[1]

[1]University of Antwerp, Belgium; [2]University of Johannesburg, South Africa; [3]University of Mpumalanga, South Africa; [4]University of Venda, South Africa

Cassava and cocoyam are dietary staples across multiple countries in Africa, where natural fermentation has long been used to improve their safety, digestibility, and flavor. While previous studies have documented changes in proximate composition and microbial counts during fermentation, the molecular-level transformations remain understudied. Untargeted metabolomics offers a way to capture these changes, though annotation rates typically remain low when relying on standard spectral matching alone.

In this work, we applied a comprehensive computational metabolomics pipeline to characterize the molecular profiles of raw and fermented cassava and cocoyam. Samples were analyzed using LC-MS/MS, and features extracted using MZmine. We then employed SIRIUS with CSI:FingerID for in silico annotation, feature-based molecular networking through GNPS, metabolic pathway analysis using mummichog, and biotransformation prediction with BioTransformer. This pipeline generated 149 unique high-confidence structural identifications and 1,158 high-confidence class classifications out of 2,452 total features with MS/MS information.

Principal component analysis showed separation between control and fermented samples for both tubers, indicating that natural fermentation alters the chemical fingerprint of both substrates. However, the two tubers responded differently (log2 fold change > 1, $p < 0.05$). In cassava, fermentation was depleting: 706 of 750 significant features were down-regulated (Figure 1). In cocoyam, the pattern was more balanced (329 up, 434 down), indicating increased metabolic complexity alongside degradation (Figure 1). Pathway enrichment also revealed distinct transformation routes; for example, chrysenes and benzoxazolones were enriched in cocoyam but absent in cassava ($p < 0.05$). Molecular networking further highlighted these differences, with spectrally related features clustering into matrix-specific families (Figure 2).

These results suggest that fermentation activates distinct microbial enzymatic pathways depending on the substrate, despite both being starchy tubers. This computational pipeline enabled a more interpretable picture of how fermentation reshapes their metabolic landscape.

Acknowledgements: This work was supported by the Research Foundation – Flanders (FWO G0AGQ24N).

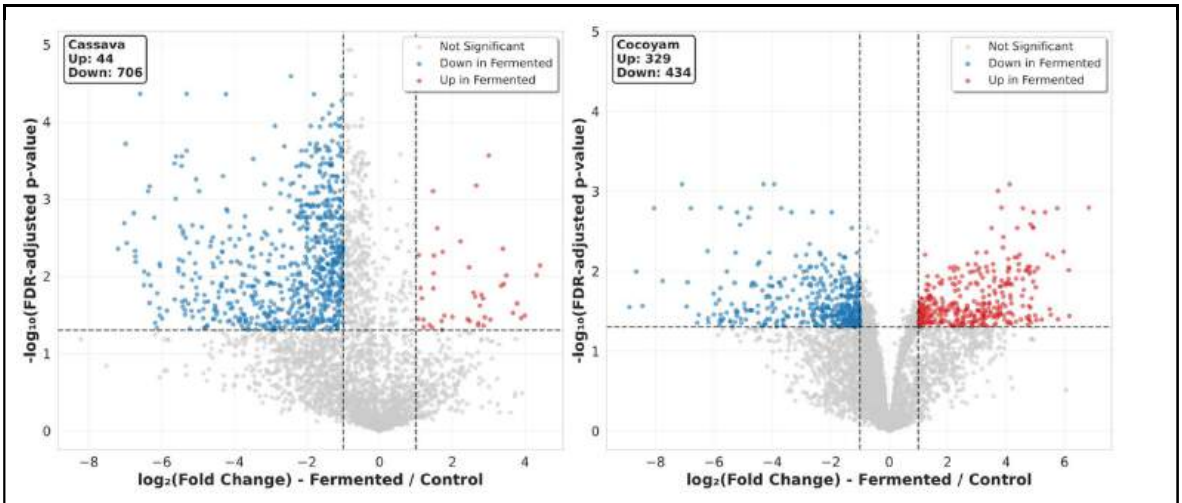

Fig. 1. Impact of fermentation on the molecular landscape of cassava and cocoyam. Cassava fermentation is predominantly depleting, while cocoyam shows a more balanced response. Volcano plots comparing fermented versus control samples in cassava (left) and cocoyam (right). Significance thresholds: |log2 fold change| > 1 and FDR-adjusted $p < 0.05$.

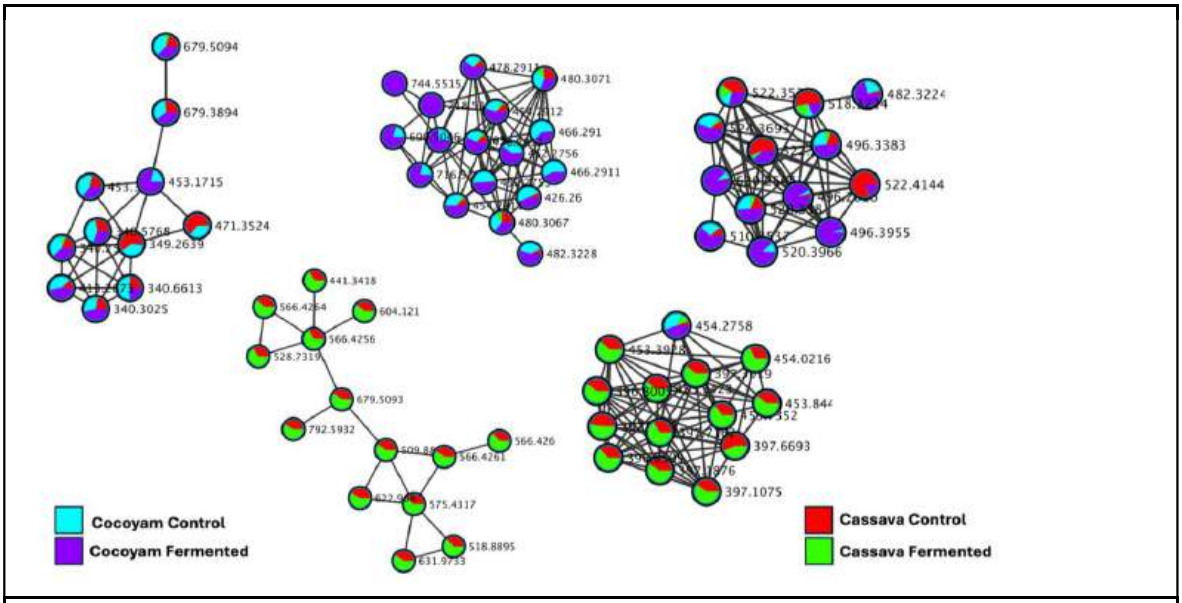

Fig. 2. Feature-based molecular networks showing compound clusters across cassava and cocoyam samples. Pie charts indicate relative abundance across conditions. Node labels represent precursor m/z values.

CBF - D1 - O07

Polyphenol–casein interactions modulate protein aggregation and network formation during curd development

Ribeiro, A.C.[1], Bravo C.[1], Brandão E.[1], Freitas V.[1], Tovar C.A.[2], Pérez-Gregorio R.[1,3,4]
[1]REQUIMTE, LAQV, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Portugal; [2]Dept. of Applied Physics, Faculty of Sciences, University of Vigo, Spain; [3]Food and Health Omics Group, Food and Agroecology Institute, University of Vigo, Spain; [4]Food and Health Omics Group, Dept. of Chemistry and Biochemistry, Galicia Sur Health Research Institute (IISGS), Spain

Polyphenols are highly reactive metabolites capable of establishing molecular interactions with milk proteins, potentially modulating protein aggregation and gel formation [1]. Although these interactions are well documented, their role in governing casein assembly and network development during milk coagulation remains insufficiently understood, particularly when polyphenols are delivered through whole food matrices.
In this study, milk curd formation was used as a control to investigate the effects of polyphenol-rich foods with distinct compositional profiles (pear, apple, blueberry, broccoli and onion) on protein coagulation, structural organization and viscoelastic behaviour. Curds were produced under acid and rennet–acid coagulation, and the resulting matrices were characterised in terms of the composition, protein recovery, molecular interactions, antioxidant incorporation and viscoelastic properties. Protein recovery and curd composition were strongly matrix and process dependent. Acid coagulation generally promoted higher protein retention, whereas rennet–acid coagulation produced weaker networks due to enzymatic hydrolysis, consistent with reported differences in casein aggregation mechanisms [2]. The incorporation of polyphenols-rich foods improved the antioxidant capacity while altering casein aggregation pathways. Fruits (apple and pear) favoured higher protein recovery, while broccoli and onion markedly modified curd structure and viscoelastic response. Spectroscopic analyses revealed phenolic-induced rearrangements in the protein secondary structure, including an increase in the hydrogen-bonded β-sheet content, particularly in broccoli and blueberry containing curds. All phenolic-enriched curds exhibited gel-like behaviour ($G' > G''$), with matrix-specific effects on stiffness, time-stability and gel quality, consistent with previous observations in polyphenol-modulated protein gels [3].Furthermore, broccoli and onion strengthened the gel networks in rennet–acid and acid curds, respectively.
These findings demonstrate that phenolic-assisted coagulation provides a matrix-driven strategy to modulate casein aggregation, curd structure and protein functionality without compromising coagulation. The results highlight the potential of plant-derived, phenolic-rich foods to tailor the nutritional, structural and viscoelastic properties of dairy protein gels through reversible, non-covalent interactions.

This work received financial support from FCT/MCTES (UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020) through national funds. The authors acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) through the PhD fellowship of Ana Catarina Ribeiro under project reference and DOI: https://doi.org/10.54499/UI/BD/153612/2022. A.C.R acknowledges financial support from the Erasmus+ programme for the placement at the University of Vigo. R.P.G would like to thank the Ramón y Cajal contract RYC2021-033224-I, funded by the Ministry of Science and Innovation and the National Agency for Research (0000421S140.06) from the ES Govern (MCIN/AEI/10.13039/501100011033) and the European Union under the frame of “NextGenerationEU/PRTR” funds. E.B. would like to acknowledge FCT for her CEEC contracts (Doi: 10.54499/CEECIND/01598/2018/CP1545/CT0004).

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CBF - D1 - O08
New insights into yeast protein–chitosan complex coacervation for food systems

Ana Rita Pereira[1], Ana Fernandes[2], Nuno Mateus[2], Victor de Freitas[2]
[1]LAQV-REQUIMTE, Portugal; [2]Faculty of Sciences, Porto University, Portugal

Soft matter physics provides a powerful framework for understanding the structural and functional complexity in food systems, including meat analogue formulations[1]. Complex coacervates are formed through liquid–liquid phase separation, driven primarily by electrostatic interactions between oppositely charged macromolecules, yielding a polymer-rich coacervate phase and a polymer-depleted supernatant phase[1]. This work proposes the formation of coacervates between yeast (*Saccharomyces cerevisiae*) protein extract (YPE) and chitosan (CH), focusing on optimizing coacervation conditions and elucidating molecular-level interactions. YPE represents a valuable protein source with a favorable amino acid profile, notably rich in branched-chain amino acids and lysine, and is recognized as safe by regulatory authorities[2]. YPE exhibited a protein content above 60%, as determined by the Kjeldahl method, and an isoelectric point at pH 3.7 revealed by ζ-potential analysis. Turbidity measurements performed at different pH values (4.0–6.0) and ionic strengths (10, 100, and 250 mM) demonstrated a pH- and CH:YPE ratio-dependent coacervation behavior. At pH 4.0 and 5.0, only minor changes in turbidity were observed upon CH addition, whereas at pH 6.0, turbidity varied significantly with the CH:YPE ratio. Optimal coacervation ratios decreased with increasing ionic strength, suggesting electrostatic interactions as the driving force for coacervate formation. Complementary analyses using isothermal titration calorimetry and FTIR spectroscopy provided further evidence of specific molecular interactions between YPE and CH. The microstructure of CH:YPE coacervates (1% w/w, optimal ratio 0.04:1), as well as of the individual biopolymers, was investigated by cryo-scanning electron microscopy to observe distinct structural features relevant for texture design in food systems. Overall, this study highlights the potential of complex coacervation to bridge chemistry and food science in the development of sustainable and rationally designed protein-based materials.

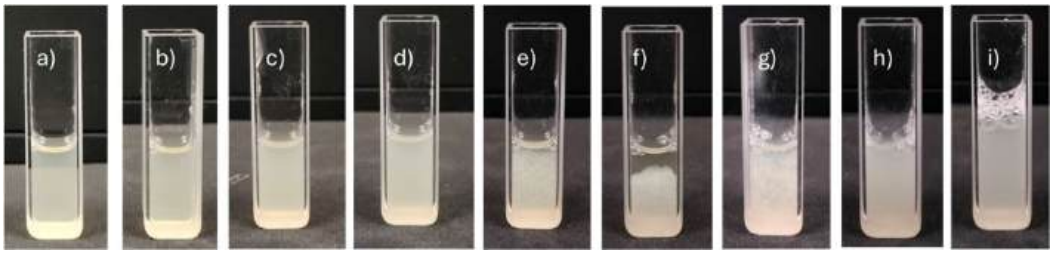

Fig. 1. Visual observation of coacervate formation in yeast protein extract (YPE 1% w/w) and chitosan (CH 1% w/w) mixtures at pH 6 for different CH:YPE ratios. Coacervate formation is indicated by the appearance of turbidity and phase separation, with variations dependent on the CH:YPE ratio. a) (0001:1); b) (0.002:1); c) (0.009:1); d) (0.01:1); e) (0.018:1); f) (0.02:1); g) (0.03:1); h) (0.05:1); i) (0.1:1).

Funding: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia, and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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CBF - D1 - O09
Prevalence and bioavailabilty of Kukoamine A and B in potatoes, potato products and peppers

Jule Fiori[1], Monika Pischetsrieder[1,2]
[1]Dept. of Chemistry and Pharmacy, Food Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; [2]FAU NeW-Research Center New Bioactive Compounds, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Kukoamine A and Kukoamine B are bioactive compounds present in commonly consumed foods originating from the Solanaceae family, such as potatoes and peppers. Several in vitro and animal studies highlight their anti-inflammatory, antioxidant, anti-diabetic and cell- and neuroprotective properties. Additionally, Kukoamines have been shown to activate human receptors, such as the μ opioid receptor.[1] Our study aims to estimate how cultivars, processing and storage influence Kukoamine concentrations in potatoes and pepper. Furthermore, their bioavailability from diet was evaluated.
We identified one pepper variety that serves as an exceptional source of Kukoamines, with concentrations up to 20 times higher than those found in typical bell peppers or potatoes. Additionally, we analyzed how storage conditions and food processing influence the stability and concentration of Kukoamines. Our results indicate that food processing at high temperatures can result in losses of more than 90%, while prolonged storage may cause reductions of up to approximately 40%.
We used LC-MS/MS to determine the levels of Kukoamines in urine after the consumption of vegetables. In a case study, we observed peak concentrations of Kukoamines four hours post-consumption. Our findings also revealed that unmodified Kukoamines are the prevalent forms detected in urine, while glucuronides and sulfates seem to play a minor role in metabolism and renal elimination.
Our results demonstrate that Kukoamine concentrations in our food highly depend on the state of storage and processing. While longer stored or highly processed foods show relatively low concentrations of Kukoamines, unprocessed vegetables seem to be our main Kukoamine source. After consumption, parts of the Kukoamines get absorbed and are subsequently excreted renally. To further assess the total amounts of Kukoamines absorbed, the metabolism and concentrations in blood should be investigated.

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CBF - D1 - O10

Sustainable NADES extraction of bioactive flavonoids from sugarcane bagasse and their antioxidant effects in *Drosophila melanogaster* Alzheimer model

Gabriela Cremasco[1], Mirella Thaisa Ferreira Ranzeti[2], Luísa de Toledo Tury[3], Joanina Gladenucci[3], Daniel Rinaldo[1,2,3], Marina Piacenti-Silva[3]

[1]Greenbiotech network, FC, Unesp, Brazil; [2]Chemistry Institute, Unesp, Brazil. [3]School of Sciences, Unesp, Brazil

Sugarcane is the second-largest agricultural crop worldwide, with Brazil being its main producer[1,2]. Despite its importance to the sugar–energy industry, the production process generates large volumes of solid waste, such as bagasse (250–280 kg per ton)[1,2]. The utilization of this by-product remains limited, despite it being a rich source of flavonoids with well-recognized antioxidant activity[3]. However, conventional extraction methods rely on toxic organic solvents, which limits its use in biology and conflicts with the principles of green chemistry. In this study, we present a sustainable approach that combines natural deep eutectic solvents (NADES) and microwave-assisted extraction (MAE) to extract bioactive flavonoids from sugarcane bagasse, evaluating their *in vivo* biological effects. Ten NADES systems were evaluated under optimized MAE conditions (50 °C for 60 minutes), and the extraction yields were quantified using HPLC-DAD and compared with those obtained using conventional methanol-based extraction. Nine of the ten NADES systems tested demonstrated higher extraction efficiency than methanol, with the betaine:glycerol (1:1 mol/mol) system proving to be the most promising. The bioactivity of the NADES-derived extract was tested in a *Drosophila melanogaster* Alzheimer's disease model using survival and locomotor performance assays in relation to the antioxidant response. Notably, the NADES extract significantly increased lifespan and improved locomotor performance, whereas the methanolic extract impaired both parameters. Combining NADES and MAE was effective in recovering flavonoids from sugarcane bagasse, delivering superior extraction efficiency and enhanced *in vivo* biological performance. These findings highlight the potential of this approach as a sustainable strategy for the valorization of agro-industrial residues, in line with global objectives.

We acknowledge financial support from CNPq, grant #303887/2024-9, and FAPESP, grants #2025/03036-3; #2025/14225-1; #2024/10984-2, Brazil.

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CBF - D1 - O11

Kinetics of reactive nitrogen species in plasma-activated water and their role in antimicrobial activity against *Escherichia coli*

Yuri Asnis, Jules Schadt, Fabio Avino, Ivo Furno
Swiss Plasma Center, École Polytechnique Fédérale de Lausanne, Switzerland

Plasma-Activated Water (PAW) is gaining attention as a promising, environmentally friendly disinfectant, with applications extending beyond microbial inactivation [1] to areas such as agriculture [2], waste-water treatment [3] and food science [4]. Despite this versatility, the underlying plasma–gas-liquid interactions that determine PAW chemistry remain challenging to resolve. Therefore, we focus on the post-discharge evolution of PAW chemistry, where reactive species exhibit liquid-phase kinetics. Using spectrophotometry, ion chromatography, and mass spectrometry, we identify nitrite (NO_2^-) and nitrate (NO_3^-) as the dominant long-lived products in our PAW. Owing to the intrinsic acidity of PAW, most of NO_2^- is present in its protonated form, HNO_2, which is thermodynamically unstable under acidic conditions and decomposes over time. This decomposition, which depends on storage conditions, can govern the temporal “tunability” of PAW, enabling distinct chemical environments that may activate different antimicrobial mechanisms. To link these chemical changes to biological effects, we evaluate the antimicrobial activity of PAW over time by treating *Escherichia coli* cultures and quantifying survivals via colony-forming unit (CFU) assays.

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CBF - D1 - O12

Antimicrobial Ionic liquid-essential oils combinations: A mathematical modelling of interactions

Utibe B. Akpan[1*], Ogechukwu V. Ezeh[2], Leslie Anne Lopez Yasis[1], Wei Han[1], King Lun Yeung[1,2]
[1]Division of Environment and Sustainability: [2]Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Hong Kong SAR, China
**ubakpan@connect.ust.hk*

The rise of antimicrobial resistance (AMR) has necessitated innovative strategies to restore the efficacy of existing antimicrobials. Combination therapy is one of those strategies.[1] This study investigated the efficacy antimicrobial combinations viz: ionic liquids (1,3-dimethylimidazolium chloride (DMIM-Cl) and 1,3-dimethylimidazolium tetrafluoroborate (DMIM-BF4)) and essential oils (carvacrol and thyme oil). Antimicrobial efficacy was assessed against drug-sensitive (*Staphylococcus aureus* and *Pseudomonas aeruginosa)* and drug-resistant (*Methicillin Resistant Staphylococcus aureus* (*MRSA)* and *Methicillin Resistant Pseudomonas aeruginosa (MRPA)*) bacteria, and the fungal spore *Penicillium rubens* with single and combined systems deposited on High Efficiency Particulate Air (HEPA) filters. In contrast to the individual components, the combinations mostly exhibited superior activity achieving > 3-log reduction in bacteria and >2-log reduction in fungal spores, with both Bliss independent and Loewe additivity models revealing concentration-and organism-dependent interactions. Figure 1 shows the interaction between carvacrol and DMIM-Cl at some specific concentration-combinations to be synergistic, additivity and antagonism with Loewe model. The higher activities of the combinations may be attributed to increased membrane permeability facilitating enhanced disruption of membrane integrity. This could have implications for developing broad-spectrum antimicrobial coatings for surfaces with enhanced efficacy to overcome antimicrobial resistance microorganisms.

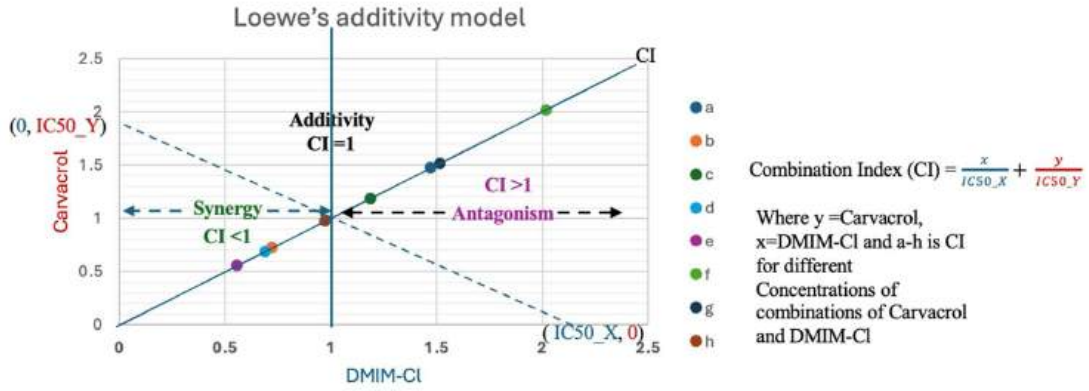

Fig. 1. Loewe's additivity model (simplified form) showing combination index (CI) of combination of carvacrol and DMIM-Cl of different concentration ratios against Staphylococcus aureus bacteria

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CBF - D1 - O15

Valorization of cocoa bean shells by green extraction: A source of functional compounds

Carlotta Valle[1], SilviaTabasso[1], Luisa Boffa[1], Giancarlo Cravotto[1]
[1]*Dept. of Drug Science and Technology, University of Turin, Italy*

Cocoa bean shells (CBS), accounting for approximately 15% of cocoa bean weight, are a major by-product of cocoa processing that has traditionally been treated as waste but is now gaining attention as a sustainable source of functional ingredients for food, cosmetic, and nutraceutical applications. This study evaluates Microwave-Assisted Subcritical Water Extraction (MASWE) as a green and efficient technology for the recovery of bioactive compounds from CBS. MASWE conditions were optimized to enhance the extraction of catechin monomers and to increase the antioxidant potential of the resulting extracts, suggesting improved bioavailability of the recovered compounds.

To further concentrate and purify target bioactives, a comprehensive screening of adsorption resins was carried out, leading to the identification of the most suitable resin for the selective recovery of polyphenols and methylxanthines. Dynamic fractionation performed on the selected resin enabled the isolation of a fraction highly enriched in these compounds, which are of growing interest for their roles in metabolic health, including antidiabetic[1] and cognitive-enhancing effects[2].

Overall, the integrated MASWE, resin screening, dynamic fractionation, and NaDES extraction approach demonstrates a scalable and sustainable valorization pathway for cocoa processing side streams, fully aligned with green extraction principles and nutraceutical innovation.

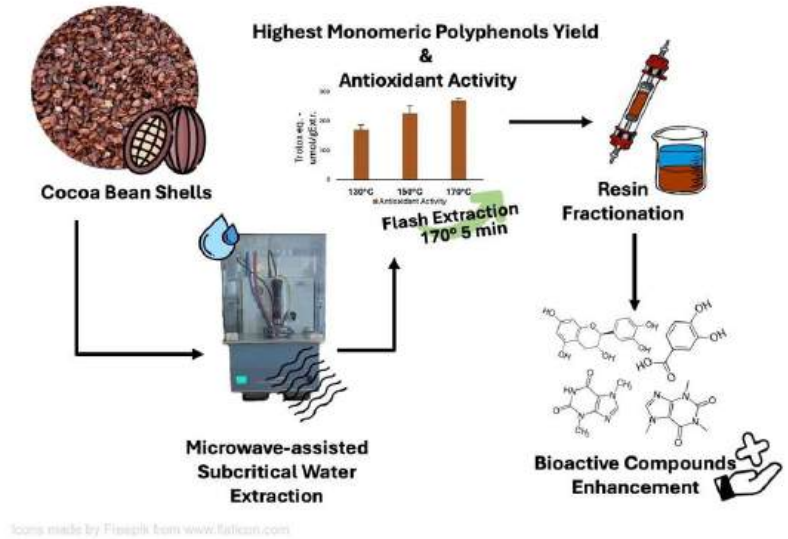

Fig. 1. Workflow scheme of extraction and downstream processing

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CBF - D1 - O16

Circular valorisation of tomato processing by-products: Recovery of bioactive compounds for sustainable food systems

Raquel Nunes da Silva[1,2], Bárbara Maurício[1,3], Ana Fernandes[1,2], Iva Fernandes[1,2], Nuno Mateus[1,2], Victor de Freitas[1,2]

[1]LAQV-REQUIMTE, Chemistry and Biochemistry Dept., Faculty of Sciences, University of Porto, Portugal; [2]Chemistry and Biochemistry Dept., Faculty of Sciences, University of Porto, Portugal; [3]Faculty of Engineering, University of Porto, Portugal

The valorisation of by-products from the tomato processing industry represents a viable and needed strategy to address global sustainability challenges by reducing agro-industrial waste and recovering high-value bioactive compounds. Rich in polyphenols, carotenoids, and other functional molecules, tomato by-products offer a sustainable resource that aligns directly with circular economy principles and the development of natural food preservation technologies.[1] In collaboration with a multinational tomato processing company in Portugal, this study explored the chemical profile of pomace from standard and high-lycopene tomato varieties and assessed their future suitability for sustainable applications in food, nutraceutical, and antimicrobial systems. Extraction and quantification of polyphenols were optimized through colorimetric assays and HPLC-DAD, enabling the tentative identification of 25 polyphenols. Carotenoids were also extracted and quantified through chromatographic and spectrophotometric approaches. Antioxidant capacity was high across both varieties, supporting their potential as natural functional ingredients to control oxidative deterioration in food products.[2] Antimicrobial assays conducted with and without light exposure further demonstrated that both polyphenol and carotenoid extracts exhibit some inhibitory effects against tomato-spoiling bacteria. Irradiation enhanced antimicrobial activity of polyphenols, highlighting their potential as natural photosensitizers for photodynamic inactivation (PDI). This work provides evidence that tomato by-products can be transformed into bioactive-rich, multifunctional ingredients suitable for sustainable food preservation and value-added applications. The optimized workflows contribute to the development of environmentally responsible solutions that simultaneously reduce waste, enhance resource efficiency, and support global efforts toward more resilient and circular food systems.

Funding: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI10.54499/UID/50006/2025 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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CBF - D1 - O17

High-throughput screening of herbal medicines for DPP-4 inhibition in type 2 diabetes mellitus using matrix-assisted laser desorption ionization time-of-flight mass spectrometry

Yu-Chi Lin[1], Chao-Jung Chen[2, 3*]

[1]Translational medicine and new drug development, China Medical University, Taichung, Taiwan; [2]Proteomics Core Laboratory, Dept. of Medical Research, China Medical University Hospital, Taichung, Taiwan; [3]Graduate Institute of Integrated Medicine, China Medical University, Taichung, Taiwan

Type 2 diabetes mellitus (T2DM) is a common metabolic disorder characterized by insulin resistance and dysfunction of pancreatic β-cells. Glucagon-like peptide-1 (GLP-1) plays a crucial role in the pathophysiology of type 2 diabetes mellitus (T2DM). It is secreted by the small intestine in response to rising blood sugar levels, promoting insulin release and protecting β-cells. However, active GLP-1 is susceptible to degradation by the enzyme dipeptidyl peptidase-4 (DPP-4), which rapidly converts it into inactive fragments. Therefore, identifying bioactive compounds that inhibit DPP-4 could prolong the activity of endogenous GLP-1, enhance its insulin-stimulating effects, and provide potential therapeutic benefits for managing type 2 diabetes. In this study, we employed matrix-assisted laser desorption ionization-time of flight mass spectrometry (MALDI-TOF MS) with a PDMS-C18 MALDI plate system[1], which is effective for rapidly desalting and removing interferences. This platform was used for high-throughput screening to discover potential DPP-4 inhibitors from 200 herbal medicines. (Figure 1) Our results showed that Galla chinensis and Taxillus chinensis exhibited over 70% inhibition of DPP-4 activity. The potential DPP-4 inhibitory compounds were successfully identified using a home-built compound database and LC-MS/MS. Furthermore, the active components responsible for DPP-4 inhibition from herbal medicines were validated using the NCI-H716 intestinal endocrine cell model. Finally, molecular docking calculations were carried out to identify potential binding sites between the compounds and the DPP-4 enzyme. This study demonstrates the effectiveness of MALDI-TOF MS-based platforms in identifying natural DPP-4 inhibitors, providing a foundation for developing novel therapeutic agents for T2DM.

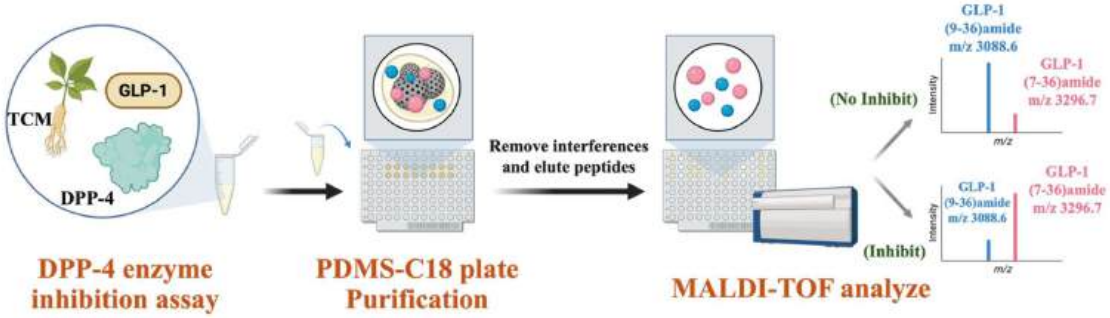

Fig. 1. The workflow for high-throughput screening of herbal medicines for DPP-4 Inhibition using a PDMS-C18 plate and MALDI-TOF analysis.

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CBF - D1 - O18

Novel heterocyclic FAT-inhibitors - Resistance-breaking and PFAS-free grass weed control solutions for sustainable agroscience in Europe

Jens Frackenpohl[1]
[1]Bayer AG, CropScience Division, Profile Driven Chemistry, Germany

The presence of weed infestations exerts considerable strain on the food production around the globe by depleting resources and facilitating the transmission of diseases. Although herbicides remain the most effective solution for weed control, they face multiple challenges, such as the emergence of resistant weed populations. Thus, it is essential that crop protection research acts rapidly to provide farmers not only with new, but sustainable and environmentally friendly solutions that enable them to control resistant weed species. In contrast to other modes of action emerging resistance against inhibitors of acyl-acyl carrier protein thioesterase (FAT, HRAC group 30) has not been observed so far making it an attractive target for identifying new herbicides. Our work outlined herein covers several novel and structurally diverse herbicidal lead structures that show good FAT-inhibition paired with strong activity against commercially important weeds (including resistant species) in broad-acre crops (e.g. wheat and corn). Our lead structures contain various new key features, e.g. [1,3]thiazolo[4,5-*b*]pyridines,[1-3] 2,3-dihydro[1,3]thiazolo[4,5-*b*]pyridines,[4,5] 1-oxa-2,7-diazaspiro[4.4]non-2-en-6-ones, 1-oxa-2,7-diazaspiro[4.5]dec-2-en-6-ones, 2,8-diazaspiro[5.5]undecane-1,7-diones,[6,7] hexahydro[3,4-b]furans[8] as well as azetidinyl and pyrrolidinyl carboxamides (Figure 1).[9] Herein, we describe how we identified and prepared these new structures involving crystal structure-based molecular modeling, modern synthetic methodology (Pd- and Fe-catalysis, Newman-Kwart rearrangement, Lewis-acid mediated hydrogenation, cycloadditions) and *in vivo*-greenhouse screening. Remarkably, these lead structures do not contain any moieties that are affected by current PFAS definitions. Thus, the use of isostere concepts to explore unusual structural features is a powerful tool to broaden the structural scope of modern agrochemical research and to address sustainability goals, e.g. overcoming herbicide resistance and meeting demanding environmental safety goals.

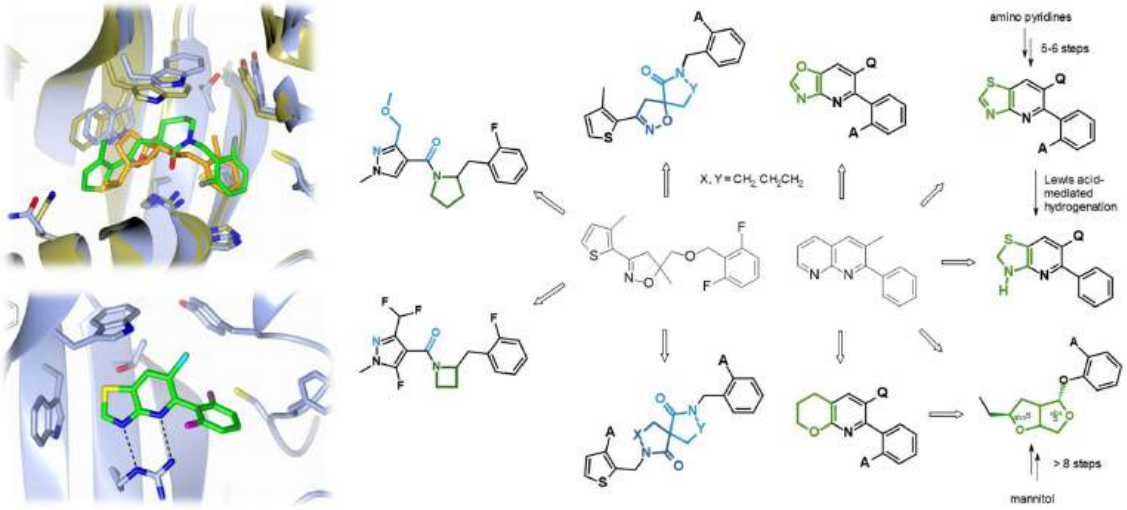

Fig. 1. New heterobicyclic herbicides inhibiting acyl-acyl carrier protein thioesterase (FAT)

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CBF - D1 - O19
LC-MS of Ovatoxins: Influence of calcium salts on ionization patterns and quantification accuracy

Chiara Melchiorre[1,2], Valeria Tegola[1], Carmela Dell'Aversano[1,2]
[1]University of Naples Federico II, Dept. of Pharmacy, Naples, Italy; [2]National Biodiversity Future Center, Palermo, Italy

Ovatoxin-a (OVTX-a) is the major palytoxin (PLTX) congener produced by the benthic dinoflagellate *Ostreopsis* cf. *ovata*[1]. Since 1990s, OVTXs are associated with toxic outbreaks and represent a growing concern for public health, as they can bioaccumulate in seafood[2]. Despite toxicological relevance of the PLTX-group of toxins, no validated analytical methods are currently available for their detection and quantification. European guidelines recommended LC-MS based methodology for determination of OVTXs in seafood[3]; however method development is particularly challenging, because of their complex molecular structures and their strong propensity to form adducts with metal ions such as Ca^{2+}, Mg^{2+}, Na^{+}, and K^{+}, which lead to poorly reproducible MS spectra complicating quantitative analysis and methods validation[4]. To date, no OVTX-a certified reference material (CRM) is available, thus LC-MS quantification of OVTX-a was performed using non-certified PLTX standard, assuming an identical molar response for PLTX and OVTX-a. However, this assumption neglects differences in ionization behavior between molecules. In this study, we systematically investigated the influence of calcium ions on the ionization patterns of PLTX and OVTX-a, in-source stability, and toxin–metal complex abundance by analyzing aqueous methanol PLTX and OVTX-a solutions added of calcium acetate (0.25 to 750 mM) under different chromatographic conditions. Preliminary results revealed differences between ionization behavior of PLTX and OVTX-a, which in turn depend on differences in their molecular structures, metal-binding affinities, and degradation pathways. Consequently, the use of PLTX as a surrogate standard for OVTX-a quantification introduces a significant risk of systematic bias. This poses the urgent need to produce OVTX-a CRM and/or to develop tailored sample preparation strategies capable of enforcing comparable metal complexation of PLTXs analogues, thereby improving the robustness and reproducibility of targeted LC-MRM-MS methods. Enhanced analytical performance directly supports more accurate marine toxin quantification, strengthening risk assessment and food safety monitoring.

Funding: Project funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 - Call for tender No. 3138 of 16 December 2021, rectified by Decree n.3175 of 18 December 2021 of Italian Ministry of University and Research funded by the European Union – NextGenerationEU. Project code CN_00000033, Concession Decree No. 1034 of 17 June 2022 adopted by the Italian Ministry of University and Research, CUP E63C22000990007, Project title "National Biodiversity Future Center - NBFC". Experimental research was funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component C2 Investment 1.1—Call for tender D.D. 104 of 2 February 2022 of the Italian Ministry of University and Research funded by the European Union—NextGenerationEU, Award Number: Project code 2022KZLJZH, Concession Decree D.D. 1015 of 7 July 2023 adopted by the Italian Ministry of University and Research, CUP I53D23003260006, Project title: Emerging toxins in Italian seas and risks for human health (Tox-IT).
Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Research Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

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CBF - D1 - F01

Cherry–carqueja functional beverage prototypes: Integrating cell bioactivity, cultivar chemistry and human metabolic biomarkers

Radhia Aitfella Lahlou[1], Filomena Carvalho[1], Luís R. Silva[1,2,3]

[1]SPRINT, Sport Physical Activity and Health Research & Innovation Center, Instituto Politécnico da Guarda, Portugal; [2]RISE-Health, Faculdade de Ciências da Saúde, Universidade da Beira Interior, Portugal, University of Beira Interior, Portugal; [3]CERES, Dept. of Chemical Engineering, University of Coimbra, Portugal

Plant beverages are increasingly investigated as convenient carriers of bioactives able to modulate inflammatory and metabolic pathways. It bridges food chemistry, in vitro biology, and prevention. We applied a biology-guided workflow to a sweet cherry juice blended with “carqueja” (*Genista tridentata*), integrating (i) cellular bioactivity and cytocompatibility, (ii) cultivar-level phytochemical context, and (iii) human biomarker evidence from whole-fruit intake.

Cell-based screening was prioritised. In LPS-stimulated RAW 264.7 macrophages, the cherry–carqueja blend reduced nitric oxide levels under a pre-treatment/co-treatment design. Cytocompatibility was assessed in parallel (RAW 264.7, NHDF and HepG2) using viability and membrane-integrity readouts to define a concentration window for formulation work.

To anchor biological effects to food chemistry, Prime-Giant cherries (Fundão, Portugal) were characterised at commercial maturity (TSS 18.13 ± 0.02 °Brix; pH 3.97 ± 0.02; titratable acidity 0.51 ± 0.01 g malic acid/100 g fresh weight). Targeted LC–MS profiling showed a phenolic fingerprint dominated by non-coloured phenolics (Σ 807.4 µg/g dried fruit) and low anthocyanins (Σ 4.6 µg/g dried fruit), mainly cyanidin 3-O-rutinoside (3.6 ± 0.071 µg/g).

Clinical translation was supported using a longitudinal single-arm pilot trial (n = 27) consuming 280 g/day Prime-Giant cherries for 42 days (baseline, day 21, day 42, and 2 weeks post-intervention). Whole-fruit intake improved long-term glycaemic control (HbA1c and estimated average glucose decreased at all time points) and inflammatory status (IL-6 and AGP-1 decreased). Oxidative stress enzymes shifted (GPx decreased at day 42 and post-intervention; GR decreased at day 42), and systemic/liver-related markers improved (LDH decreased by day 42; GGT decreased two weeks post-intervention).

In conclusion, linking cell bioactivity and safety with cultivar chemistry and human biomarker signals supports cherry–carqueja beverages as food-grade functional prototypes and motivates standardised phenolic specifications and controlled follow-up trials.

Acknowledgments: The work was performed with the support of the Local Health Unit of Guarda (ULS Guarda), the company CerFundão (Fundão) and the laboratory Egianálise (Guarda).

Funding: This work was funded by the Programa Operacional Regional do Centro (CEN-TRO-04-3559-FSE-000162) within the European Social Fund (ESF), CICS-UBI (UIDP/00709/2020) financed by National Funds from Fundação para a Ciência e a Tecnologia (FCT), Community Funds (UIDB/00709/2020), by Fundação La Caixa and Fundação para a Ciência e Tecnologia (FCT) under the Programa Promove Project PD21-00023 (PharmaStar) and supported by project PRR-C05-i03-I-000143 (RedFruit4Health), by Project RedSup4Health - COMPETE2030-FEDER-01451300, operation number 18308, and by Project Red4Cardio - COMPETE2030-FEDER-00794300, operation number 16761.

CBF - D1 - F02
Geographical fingerprinting of wine: Multi-technique approach and signal masking effects

Raffaello Nardin[1,2], Duccio Tatini[1,2], Alessandro Cavaglioni[1], Marco Consumi[1,2], Gabriella Tamasi[1,2], Claudio Rossi[1,2]
[1]Dept. of Biotech. Chem. and Pharma, University of Siena, Italy; [2]CSGI, Polo Scientifico Sesto Fiorentino, Italy

In the recent years, multiple analytical strategies have been proposed to gain insights on provenance to obtain reliable regional and sub-regional zoning. However, many of these techniques either rely on markers that are tied to both biotic and abiotic factors (e.g. volatile and semi-volatile [1] profiling) or tied to geological composition of the soil rather than specific geographical provenance (e.g. $^{87}Sr/^{86}Sr$ [2]). Furthermore, the addition of chemicals during the vinification process such as exogenous tannins and bentonites can further remove the specific correlation between provenance and finished product [3].
Here, in order to detangle the possible overlap of multiple signals and to gauge the robustness of each approach, the same wine dataset was analyzed with multiple complementary techniques. Each analytical dataset was first assessed independently to determine the zoning capabilities at a regional and sub-regional scale and was used to create either univariate or multivariate models. Each classification performance was then compared, and particular attention was given to the possibility of merging datasets together to increase the zoning capabilities, using a feature-level data fusion approach. Furthermore, on selected wines, the impact of winemaking practices on geographical signal preservation was investigated, evaluating the potential of well-known and used additives to introduce unwanted noise in both the elemental profile and the isotopic fingerprint of the finished product.
Results show that despite significant variation in the elemental composition introduced by winemaking practices, levels of elements tied to isotopic fingerprints do not vary significantly, making it a reliable choice for zoning efforts. Moreover, zoning capabilities of the isotopic markers improve significantly when combined with other fingerprints, particularly ICP-MS data.

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CBF - D1 - F03

Portable multiplex quantification of marine biotoxins via digital colour-encoded lateral flow platform utilizing shape-tailored gold nanoparticles

Perveen Akhtar[1,2], Hugh J. Byrne [2], Furong Tian[1,2], Bilal Javed[1,2*]
[1]School of Food Science and Environmental Health, TU Dublin Grangegorman, Ireland; [2]Physical to Life Sciences Research Hub, TU Dublin, Ireland

Shellfish and fish are vital sources of protein and nutrition, but in certain circumstances, they accumulate marine biotoxins that cause high numbers of intoxications in humans every year. Different assays are available for the detection of these toxins, but these methods involve complex sample preparation and limitations in sensitivity and specificity. Therefore, there is a growing need for rapid detection, such as multiplex lateral flow immunoassays (LFIA), capable of simultaneously detecting multiple toxins with improved sensitivity and specificity to address practical challenges in seafood testing and monitoring due to their cost-effectiveness and scalability. For the development of the LFIA strip, gold nanoparticles (AuNPs) of varying morphologies were synthesized using the Turkevich method, hydroquinone-mediated seeded growth (via 15 nm Au seeds), and a seedless approach employing increasing buffer ratios (R = [HEPES]/[$HAuCl_4$]). As a result, Spherical AuNPs of 21 nm and 40 nm (red), Au nanopopcorns of 150 nm, Au Nanostars of 60 nm (blue) and 140 nm (purple), and Au Nanoflowers of 98 nm (blue) and 122 nm (purple) were synthesized and characterized using UV–Vis spectroscopy, DLS, and SEM. For antibody conjugation, the optimal pH and antibody concentration were determined via checkerboard titration. The target toxin was conjugated to BSA (carrier protein), and the conjugation was confirmed using FTIR and NMR spectroscopy. LFIC test strips were assembled, biochemically optimized, and validated using spiked samples. To enable on-site quantification, a mobile application was developed using Python programming and Streamlit, providing both single (tetrodotoxin, brevetoxin, domoic acid, okadaic acid) and multiplex detection modes. The app allows users to upload LFIC strip images and applies four-parameter logistic (4PL) and logistic regression models to convert color intensity into quantitative toxin concentrations, indicating whether values exceed or fall below EU regulatory limits.

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CBF - D1 - F04

In vitro testing of antifungal biocides against endophytic fungi of cork oak with potential phytosanitary application

Raquel Nunes da Silva[1,2], Ana Luísa Capela Ribau[3], Ângela Cunha[3,4], Nuno Mateus[1,2], Victor de Freitas[1,2]
[1]LAQV-REQUIMTE, Chemistry and Biochemistry Dept., Faculty of Sciences, University of Porto, Portugal; [2]Chemistry and Biochemistry Dept., Faculty of Sciences, University of Porto, Portugal; [3]Dept. of Biology, University of Aveiro, Campus Universitário de Santiago, Portugal; [4]Dept. of Biology & CESAM, University of Aveiro, Campus Universitário de Santiago, Portugal
Corresponding author: raq.silva@fc.up.pt

The cork oak (*Quercus suber* L.) is a species of high ecological and economic importance in the Mediterranean region, particularly in Portugal [1,2]. Climate change has intensified the incidence of fungal diseases, notably those caused by *Biscogniauxia mediterranea*, the causal agent of charcoal canker, and *Diplodia corticola* [3,4], responsible for canker formation, both of which negatively affect tree vitality and cork production.
The primary objective of this work was to validate an experimental design for assessing the antifungal activity of different biocides, namely copper oxychloride, graphene oxide (GO) and a phenolic compound. Given the endophytic nature of the fungi under study, particularly *B. mediterranea*, spore extraction under laboratory conditions proved challenging, requiring prior optimization of growth conditions.
Different fungal growth methodologies were therefore evaluated, including the assessment of radial growth on various culture media and the application of a double-layer method incorporating antifungal agents, with growth monitored over a 7-day incubation period. In parallel, exploratory assays were conducted to obtain spore suspensions.
These assays enabled the evaluation of the antifungal efficacy of the different biocides against the two pathogenic species under study. Overall, the methodology proved suitable for assessing antifungal activity, yielding promising phytosanitary control results against both fungal species.

Funding: The authors thank Prof. Teresa Lino-Neto (Dept. of Biology, Centre of Molecular and Environmental Biology, School of Sciences, University of Minho) for providing the fungal isolates. This work was funded by national funds through FCT – Fundação para a Ciência e a Tecnologia, I.P., under the project CESAM – Centre for Environmental and Marine Studies, references UID/50017/2025 (https://doi.org/10.54499/UID/50017/2025) and LA/P/0094/2020 (https://doi.org/10.54499/LA/P/0094/2020). Additional financial support was provided by Portuguese national funds (FCT/MECI – Fundação para a Ciência e Tecnologia and the Ministry of Education, Science and Innovation) through the project UID/50006/2025 (https://doi.org/10.54499/UID/50006/2025), associated with the Associate Laboratory for Green Chemistry – Clean Technologies and Processes. This work was also developed within the scope of the Cut&Care GP project (reference 2023.16151.ICDT), which received the DOI https://doi.org/10.54499/2023.16151.ICDT.

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CBF - D1 - F05

From Mediterranean agri-waste to functional molecules for food packaging and dermo-cosmetic applications: Process-driven sustainable and circular chemistry

Francesco Cairone[1*], Laura Di Muzio[1], Simone Carradori[2], Stefania Petralito[1], Patrizia Paolicelli[1], Stefania Cesa[1]

[1]Dept. of Chemistry and Technologies of Drug, "La Sapienza" University of Rome, Italy; [2]Dept. of Pharmacy, "G. d'Annunzio" University of Chieti-Pescara, Italy

Mediterranean agro-industrial residues are an abundant and underexploited source of structurally different natural compounds. This work presents an integrated research platform aimed at transforming biomasses into high-value molecules and materials through process-oriented green chemistry.

Two different largely available co-products, such as *Punica granatum* peels and *Opuntia ficus-indica* cladodes, both coming by high draw resistant Mediterranean species, were used. These were selected as representative case studies due to their enormous availability and richness in phytochemical composition. Beyond conventional extraction, the project explores intensified and tunable methodologies such as ultrasound-, microwave-, and supercritical CO_2-assisted extraction to control mass transfer, reduce solvent consumption, and selectively recover target phytochemicals. These techniques are being comparatively optimized to establish scalable protocols with improved efficiency–sustainability balance. These co-products are rich of bioactives, such as ellagitannins in pomegranate peels [1], and piscidic acid and flavonoid derivatives in *Opuntia* residues [2], confirming these waste products as a significant reservoir of antioxidant metabolites.

The recovered fractions were applied across multiple domains: antioxidant and anti-inflammatory formulations for dermo-cosmetic use, bioactive systems exploiting the wound-healing potential of phenolic constituents, and biodegradable materials. Moreover, structural biomass components were simultaneously valorized to produce cellulose- and polysaccharide-based composites, yielding active packaging films with enhanced mechanical performance and intrinsic antioxidant functionality.

This multi-stream strategy demonstrates how a single agricultural waste can be fractionated into complementary outputs (functional molecules, biomedical ingredients, and sustainable materials) providing a model of circular chemistry in which extraction science, natural product chemistry, and materials engineering converge toward zero-waste biorefineries.

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CBF - D1 - F06

Chemistry-to-biology translation for functional fruit beverages: A comparative pipeline for *Sorbus*, *Viburnum tinus* and *Rhus coriaria* hot-water infusions

Radhia Aitfella Lahlou[1], Luís R. Silva[1,2,3]

[1]SPRINT, Sport Physical Activity and Health Research & Innovation Center, Instituto Politécnico da Guarda, Portugal; [2]RISE-Health, Faculdade de Ciências da Saúde, Universidade da Beira Interior, Portugal; [3]CERES, Dept. of Chemical Engineering, University of Coimbra, Portugal

Plant-based beverages are increasingly explored as food-compatible carriers of bioactives that may modulate oxidative and inflammatory pathways [1,2]. We compared hot-water fruit infusions from three underused/culturally established resources from Serra da Estrela (Portugal): wild *Sorbus* (*S. aucuparia*, SA; *S. latifolia*, SL), laurustinus (*Viburnum tinus*), and sumac (*Rhus coriaria*), integrating activity fingerprints (DPPH•, $O_2^{\bullet-}$, •NO scavenging, and *α*-glucosidase inhibition) with cell-based evidence (MTT/LDH in NHDF and RAW 264.7). Across berry infusions, *V. tinus* combined high phenolics (313.840 ± 8.388 mg GAE/g) with the strongest *α*-glucosidase inhibition (IC_{50} = 2.778 ± 0.0819 µg/mL) and DPPH• scavenging (IC_{50} = 4.646 ± 0.084 µg/mL). *R. coriaria* ranked next for *α*-glucosidase (IC_{50} = 7.44 ± 0.38 µg/mL) and DPPH• (IC_{50} = 12.62 ± 0.33 µg/mL) and showed the best •NO scavenging (IC_{50} = 55.17 ± 1.70 µg/mL). For *Sorbus* berries, SL contained higher phenolics than SA (269.124 ± 6.325 vs 42.117 ± 6.200 mg GAE/g DW), yet SA showed stronger radical scavenging (DPPH• IC_{50} = 35.663 ± 0.123; $O_2^{\bullet-}$ IC_{50} = 15.236 ± 0.148 µg/mL) than SL (DPPH• 157.323 ± 0.547; $O_2^{\bullet-}$ 86.263 ± 0.125 µg/mL); both were weak for α-glucosidase (SL 356.862 ± 0.362; SA 405.040 ± 4.581 µg/mL) and •NO scavenging (SL 885.458 ± 48.256; SA 713.588 ± 39.426 µg/mL). In NHDF, *Sorbus* was tolerated up to ~200–450 µg/mL; *R. coriaria* was biocompatible at 50–200 µg/mL; and *V. tinus* was weakly cytotoxic. In RAW 264.7, *Sorbus* became cytotoxic from ~200–400 µg/mL, so LPS–NO suppression was most interpretable at ≤50–100 µg/mL; *R. coriaria* maintained >80% viability at 25–200 µg/mL and strongly reduced LPS–NO at 800 µg/mL; *V. tinus* reduced NO at 400–800 µg/mL but showed emerging cytotoxicity at 800 µg/mL. Overall, activity fingerprints aligned, sometimes imperfectly, with cytotoxicity-gated anti-inflammatory signalling, supporting rational selection of fruit-derived ingredients for food/health interfaces.

Funding: This work was funded by the Programa Operacional Regional do Centro (CEN-TRO-04-3559-FSE-000162) within the European Social Fund (ESF), CICS-UBI (UIDP/00709/2020) financed by National Funds from Fundação para a Ciência e a Tecnologia (FCT), Community Funds (UIDB/00709/2020), by Fundação La Caixa and Fundação para a Ciência e Tecnologia (FCT) under the Programa Promove Project PD21-00023 (PharmaStar), by Project RedSup4Health - COMPETE2030-FEDER-01451300, operation number 18308, and by Project Red4Cardio - COMPETE2030-FEDER-00794300, operation number 16761.

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CBF - D1 - F07
Sustainable scale-up of fatty acids and polyphenols extraction from spent coffee grounds

Carmen Corea[1], Robert Hartmann[2], Laura Riva[1], Laura Gallo[3], Carlo Punta[1]
[1]Politecnico di Milano, Italy; [2]Fraunhofer-Zentrum für Chemisch-Biotechnologische Prozesse CBP, Germany; [3]Coffeefrom Srl, Italy

Approximately 20 million tons of Spent Coffee Grounds (SCG) are generated each year as a by-product of the brewing process, therefore the identification of potential applications for SCG is of great importance to reduce the environmental impact of the entire supply chain. Despite source-dependent variations, generally dry SCG contains a non-negligible amount of bioactive compounds, including polyphenols and diterpenes (≈3-5%), within a consistent share of lipids (≈20%). It also contains cellulose and hemicellulose, lignin and proteins[1].
This study focuses on the sustainable extraction and utilization of fatty acids and bioactive compounds.
The EthaNa process[2] represents an alternative approach to traditional extraction with organic solvents, since it is performed at ambient pressure and temperatures lower than 70°C, with the possibility to recycle the solvent. The application of this process to SCG has been investigated and optimized in terms of extraction yields to recover the fatty acid fraction in the pilot-scale plant of Fraunhofer CBP in Leuna.
Additionally, the potentiality of the process has been investigated at laboratory-scale by testing different solvents in sequence, including other organic solvents and NADES (natural deep eutectic solvents), aiming at a more selective extraction of polyphenols.
Fatty acid and oils find application in a variety of different fields[3], and the solid residue can be further processed to obtain high-added value products[4] or be used as it is in polymer compounding with better performances than SCG[5].
Promising results have been observed, especially considering that the scale of the process allows an effective integration of this valorization step in the supply chain.

Fig.1. EthaNa Process Scheme

The author wishes to thank Coffeefrom Srl, Fraunhofer institute and the European Union NextGeneration EU (National Recovery and Resilience Plan_NRRP): Mission 4, Component 2, Investment 3.3_DM n. 630/2024 for the funding and facilities.

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CBF - D2 - O01

Lipopolysaccharides for modulation of innate immunity receptors: The computational eye

Marina Mínguez-Toral[1], Gema Fernández-Vasco,[1] Olmo Martín-Cámara,[1] Manuel Fresno,[2] Alba Silipo,[3] Antonio Molinaro,[3] Flaviana Di Lorenzo,[3] Sonsoles Martín-Santamaría[1]

[1]Center for Biological research Margarita Salas, CSIC, Spain; [2]University Autonoma of Madrid, Spain; [3]University Federico II of Naples, Italy

In the immunotherapy era, Toll-like receptors (TLRs) are key therapeutic targets due to their primordial role in the activation of the innate immunity through the recognition of pathogen-associated molecular patterns. Deep structural understanding of TLRs signalling and mechanism is leading to the discovery of novel molecules with desirable therapeutic properties as anti-inflammatory agents or vaccine adjuvants, with already some TLR modulators used in cancer therapy, and several candidates in clinical phases.[1,2] We have addressed the computational characterization of the assembly of activated TLR models (TLR4/TLR4, TLR4/TLR2, TLR2/TLR1, and TLR2/TLR6), and the study of the molecular recognition processes of agonist and antagonist TLR modulators, ranging from atypical lipopolysaccharides (LPS) to glycolipids and small molecules with drug-like structure, for the design and discovery of novel modulators.[1,2,3,4]

In particular, we have investigated the immune modulation mechanisms elicited by LPS from representative members of the oral and gut microbiota with different behaviours depending on the chemical structure (Figure 1).[2] We have also focused in the LPSs from the opportunistic *Ochrobactrum* sp. and their different ability to bind/activate TLR4/TLR2 depending on the chemical structure of lipid A *vs* core carbohydrate composition.[5]

We combine different computational techniques (protein-protein and ligand-protein docking, multiscale molecular dynamics (MD) simulations, accelerated MD simulations, membranes simulation, machine learning (ML)-based techniques) with experimental data, chemical synthesis and biological assays.

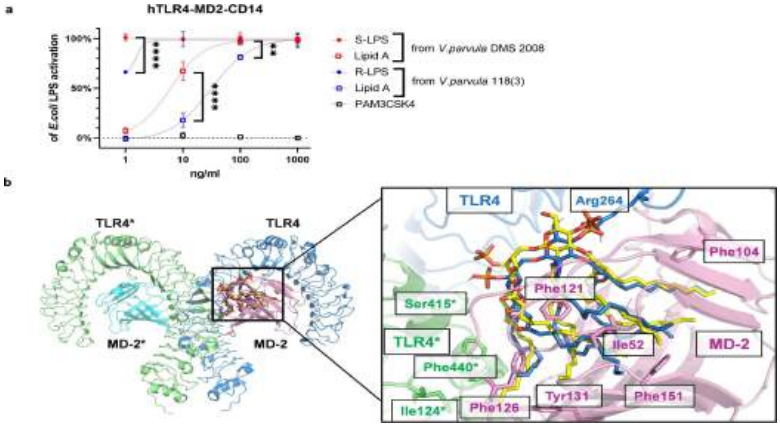

Fig. 1. TLR4 activation by *Veillonella parvula* LPS.

Acknowledgements: PID2023-152271NB-I00.

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CBF - D2 - O02

Mannosylated peptide nanofibers for MUC1-mimetic antigen delivery and immune modulation

Andrea Sodini[1], Silvia Fallarini[2], Filippo Susini[1], Gaia Lesca[3], Silvia Scaglione[3], Maria Elisabetta F. Palamà[3], Francesca Maestrelli[1], Maria Cristina Salvatici[4], Federica Cefalì[1], Mustafa O. Guler[5], Ayse Begum Tekinay[6], Cristina Nativi[1]

[1]Dept. of Chemistry, DICUS, University of Florence, Italy; [2]University of Piemonte Orientale, Dept. of Pharmaceutical Sciences, Italy; [3]React4Life S.p.A., Italy; [4]Institute for the Chemistry of Organometallic Compounds (CNR-ICCOM), Italy; [5]The Pritzker School of Molecular Engineering, The University of Chicago, USA; [6]Requalite GmbH, Hans-Cornelius, Germany

Tumor Associated Carbohydrate Antigens (TACAs) can be successfully employed to precisely modulate immune responses, including directing monocyte-derived dendritic cells. Mannosylated peptide nanofibers (Man-PA) are engineered biocompatible platforms able to pass through cell membranes and endowed with immunomodulating properties.

Merging the properties of nanofibers and TACAs, self-assembled Man-PA were prepared and functionalized with a validated MUC1, namely TnThr mimetic (Tn-MIM), to promote dendritic cell maturation and differentiation (Figure 1).[1,2]

The resulting Man-PA/Tn-MIM nanofibers exhibited robust cell-penetration properties and facilitated efficient presentation of the antigen mimetic, leading to enhanced recruitment of lymphocytes, invariant natural killer T (iNKT) cells, and natural killer (NK) cells. Importantly, these nanofibers skewed the immune response toward a Th1 phenotype, supporting both cellular and humoral immunity.

Organ-on-chip studies further validated the cytotoxic potential of lymphocytes activated by dendritic cells exposed to Man-PA/Tn-MIM. Collectively, these results provide a foundation for designing more targeted immunotherapies while minimizing complications associated with heterogeneous antigen presentation and adjuvant use. [3]

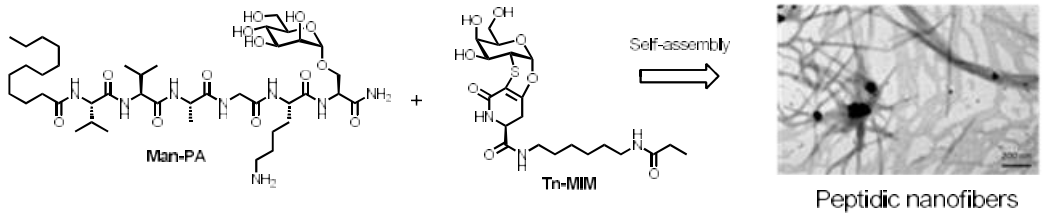

Fig. 1. Structure of Man-PA and Tn-MIM; TEM image of self-assemble Tn-MIM nanofibers.

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CBF - D2 - O03

Enzymatic and subcritical water extraction based strategies to increase psychobiotic activity through cell wall polysaccharide modulation

Soraia P. Silva[1], Sónia S. Ferreira[1], Rita Bastos[2], Mariana Mota[1], Maria H. Luís[1], Andreia F. Salvador[3,4], Maria J. Alegria[5], Sónia Mendo[6], Clarisse Nobre[3], Manuel A. Coimbra[1], and Elisabete Coelho[1,*]
[1]LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Portugal; [2]Colab4Food – Collaborative Laboratory, INIAV - Vairão, Portugal; [3]CEB–Centre of Biological Engineering, University of Minho, Portugal; [4]LABBELS –Associate Laboratory, Portugal; [5]SUMOL COMPAL Marcas S.A, R., Portugal; [1]CESAM, Dept. of Biology, University of Aveiro, Portugal

Soluble polysaccharides and oligosaccharides are prebiotic compounds that promote the growth of beneficial gut bacteria and contribute to improved health. Industrial juice production results in juices with moderate amounts of soluble dietary fibre because most polysaccharides that constitute the dietary fibre are retained in pulp (41-37%), mostly insoluble fibre rich in cellulose and pectic polysaccharides. Incorporation of glucanases and pectinases into the juice production process can therefore enrich the juice with soluble fibre and possible prebiotic effects. Apple cloudy juice was composed of 4% of fibre (dry basis), mainly pectic polysaccharides. Hydrolysis of apple pulp with endo- and exo-cellulase released a high amount of material (63.9%), composed of monosaccharides and cellulose and xyloglucan oligosaccharides. Hydrolysis with pectin lyase, polygalacturonase, and pectin methylesterase released 57.7% material composed of pectic poly- and oligosaccharides. Fermentation with fecal inocula, increased the concentration of short-chain fatty acids (SCFAs), γ-aminobutyric acid (GABA), and 5-hydroxytriptophan. Enzymatic treatment with pectinases improved the intestinal microbiota and the production of neurotransmitters.
In lignified by-product materials, more drastic strategies need to be used to recover polysaccharides and oligosaccharides with prebiotic activity. Pine nut skin, a by-product obtained during pine nut processing, is a source of insoluble dietary fiber[1,2]. Subcritical-water extraction allowed to obtain an extract rich in pectic polysaccharides and xyloglucans[1] that had an impact on the microbiota composition similar to fructooligosaccharides used as positive control, also increasing the abundance of *Bifidobacterium adolescentis*. The core microbiome upon these polysaccharides' fermentation was composed of multiple butyrate producers, which lead to butyrate increase. A selective microbial utilization towards xyloglucans was observed in detriment of pectic polysaccharides, attaining the highest GABA concentration at 24h. Pine nut skin can be considered a source of soluble oligo- and polysaccharides with prebiotic effect, promoting the growth of psychobiotics which may help reduce depression, anxiety, and modulate mood.

Acknowledgments: This work was funded by VIIAFOOD-1.2.2. FFV Fruit Fractioning and Valorization from PRR (Programa de Recuperação e Resiliência). Authors acknowledge the FCT financial support through MoodFood project (COMPETE2030-FEDER-00744200, https://doi.org/10.54499/2023.16749.ICDT) within the COMPETE 2030 and UID/50006/2025 LAQV/REQUIMTE within the PT2020 Partnership Agreement, thank FCT/MCTES for PhD grant (SFRH/BD/136471/2018), and research contracts (DL 57/2016/CP1482/CT0038, https://doi.org/10.54499/2023.08855.CEECIND/CP2840/CT0027).

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CBF - D2 - O04
Expeditious synthesis of glycan and glycopeptides and their use in pathogen detection

Mattan Hurevich[1]
[1]*The Hebrew University of Jerusalem, Israel*

Glycosylation of proteins, as well as sialylation and sulfation of glycans, plays a role in modulating cellular interactions, guiding pathogenicity, and influencing the effectiveness of antiviral and antibacterial drug treatments. Glycoconjugates have huge potential in providing fast and accurate detection of pathogens and in determining treatment efficacy in healthcare and food applications. The difficulty in gaining access to complex glycoconjugates, their low-affinity interactions, and the effect of modifications on binding hampers attempts to develop robust sensing technologies. I will describe automated and solid-phase approaches that expedite and optimize the synthesis of glycans and glycopeptides.[1,2] I will show how electrochemical biosensors made by surface-anchored glycoconjugates enable pathogen profiling. I will demonstrate that the combination of glycan modifications and surface variations serves to increase the dataset quality and the differentiation between pathogens. I will focus on insights into structural and binding preferences that are gained by surface analysis techniques. The application of glycan-based biosensors in detecting viral and bacterial infections in cell growth media and in food samples will be highlighted.[3] Finally, I will share a new concept in which single-walled carbon nanotubes functionalized with modified monosaccharides serve as the basis for enantioselective volatile organic compound gas sensing.[4]

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CBF - D2 - O05
Designing multivalent glycofullerenes for redox-active lectin biosensors

Gema Nieto-Ortiz[1], Gonzalo Gómez-Mínguez[1], Nazario Martín[1,2], M. Ángeles Herranz[1], Beatriz M. Illescas[1]
[1]Universidad Complutense de Madrid, Spain; [2]IMDEA Nanociencia, Spain

Multivalent lectin-carbohydrate interactions play a central role in pathological processes ranging from viral entry to tumor progression. However, their efficient detection remains a major challenge for advanced biosensing. Carbohydrate-functionalized [60]fullerene hexaadducts (glycofullerenes) have proven effective and selective in lectin recognition, and our research group has reported glycofullerenes that inhibit viruses such as Ebola, Zika,[1] and SARS-CoV-2.[2]
Herein, we report the design of three glycosylated fullerene-based nanoplatforms that integrate multivalent carbohydrate recognition with redox-active signal transduction for electrochemical protein sensing. Asymmetric mannose-functionalized glycofullerenes were synthesized and conjugated through CuAAC click chemistry to anthraquinone (AQ) and π-extended tetrathiafulvalene (exTTF), the latter previously established in our studies as a reliable redox probe in biological environments.[3]
In addition, we prepared a distinct [60]fullerene hexakis-adduct platform engineered to undergo three orthogonal click reactions. This unique architecture enables the controlled and sequential incorporation of ten mannose units for enhanced multivalent recognition, one exTTF moiety as a redox-active center, and a pyrene unit for anchoring onto carbon electrodes.
The resulting nanostructures are water-soluble and modular, integrating molecular recognition and signal transduction in a unified design. These redox-active glycofullerenes provide a versatile strategy for next-generation electrochemical biosensors targeting protein recognition.

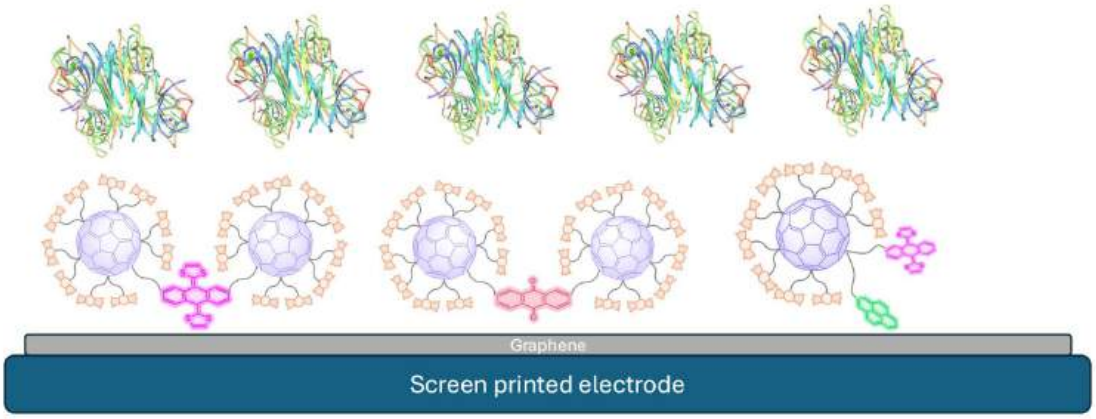

Fig. 1. Redox-active glycofullerenes for protein biosensing.

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CBF - D2 - O06
Synthesis & development of mucus-derived glycans as novel anti-virulence therapeutics

Carmen R. Cori[1], Giulietta Minzer[1], Alem Storani[1], Victoria Susan[1], Haris Majstorović[1], Rachel Hevey[1]
[1]*University of Basel, Switzerland*

Glycans (*i.e.*, carbohydrates) are an important family of natural products which coat all cell surfaces and play essential roles in cell signaling and function. Many diseases are characterized by changes in glycan structures, suggesting their potential utility as a therapeutic target.
The mucosal barrier is well-established to play an important role as a first line of host defense. Although this has traditionally been attributed to the physicochemical properties of mucus, recent reports indicate that mucin glycoproteins (the main protein component of mucus) and their associated glycans can regulate gene expression and are capable of attenuating virulence in diverse, cross-kingdom pathogens, including Gram-positive bacteria, Gram-negative bacteria, and fungi.
With mucins displaying several hundred distinct glycans, we sought to identify the discrete glycan structures responsible for this virulence regulation. Individual mucin O-glycans are not commercially available, are not amenable to automated synthesis, and given their overlapping physical and chemical properties cannot be isolated as pure compounds from natural sources using current technologies.
Therefore, through a multi-center collaborative effort (full list of contributors in ref[1-4]) we have been: (i) characterizing complex mucin O-glycan mixtures to identify structures most likely to display virulence-regulating activity; (ii) developing a synthetic approach to obtain individual mucin O-glycans in sufficient quantity for functional analysis[1,2]; and (iii) assessing the virulence attenuating capabilities of individual glycans in diverse pathogens[3,4]. Within this framework, we have successfully identified specific structures that suppress virulence phenotypes in fungal pathogen *Candida albicans* (*e.g.*, filamentation, biofilm formation), and regulate pathogenicity in *Vibrio cholerae* (*e.g.*, reduced cholera toxin production), with potency comparable to native mucin glycan pools.

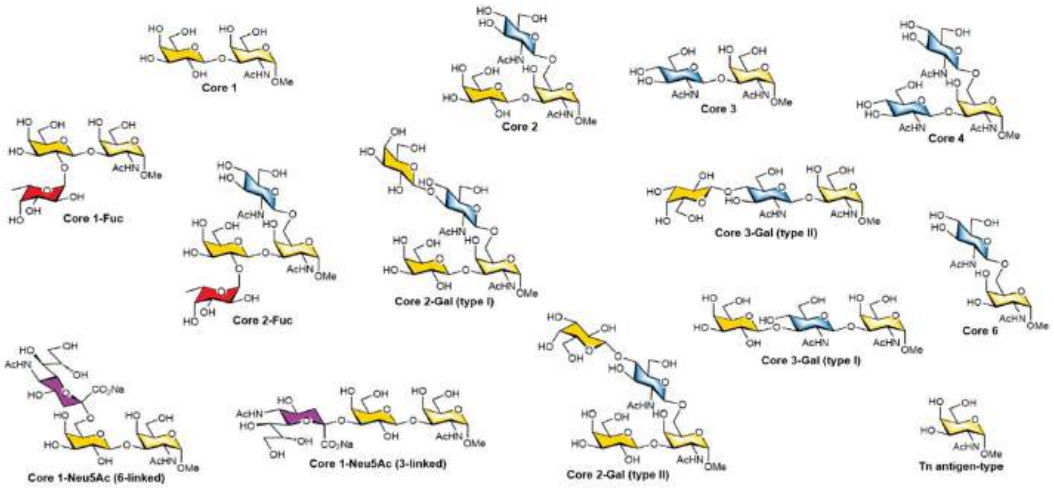

Fig. 1. Examples of synthesized mucus-derived glycans of interest for regulating pathogen virulence.

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CBF - D2 - O07
Chemical profiling of virulence-related bacterial proteases

Michaela Prothiwa
University Antwerp, Belgium

Antibiotic resistance is rising worldwide, creating an urgent need for new strategies to treat bacterial infections. One promising alternative to traditional antibiotics is to block bacterial virulence, the mechanisms bacteria use to damage the host, rather than targeting bacterial survival. This approach may slow the development of resistance.
Bacterial proteases are key virulence factors. They help pathogens evade the immune system and establish chronic infections. Despite their importance, it is often unclear which proteases are catalytically active during infection and how their activities contribute to disease, limiting their evaluation as drug targets.
In this presentation, I will discuss recent, unpublished work from my research group that addresses this problem using activity-based probes (ABPs). ABPs are small molecules that selectively react with enzymes only when they are catalytically active. This allows us to directly measure protease activity in complex, infection-relevant settings. We focus in particular on extracellular bacterial proteases. Because these enzymes act outside the cell, they are readily accessible to chemical probes and inhibitors, making them especially attractive targets for drug and diagnostic development.
As an example of this approach, we study IgA1 proteases (IgA1Ps) from *Haemophilus influenzae*, which disable human antibodies at mucosal surfaces. Using substrate-mimicking peptides equipped with serine-reactive warheads, we developed ABPs that selectively label *H. influenzae* IgA1Ps with minimal cross-reactivity toward other bacterial or human proteases, even in complex samples. These probes enabled profiling of native IgA1Ps across *H. influenzae* clinical isolates and revealed pronounced heterogeneity in IgA1P activity, identifying strains with particularly high immune-evasive potential. Using the probes in competitive screening experiments, we identified potent inhibitors that block IgA1 cleavage and restore IgA1 binding on the bacterial surface of these high-activity isolates, thereby counteracting this immune evasion mechanism.
Overall, this work highlights ABPs as powerful chemical tools for identifying and validating druggable bacterial virulence factors.

CBF - D2 - O08
Targeting RNA with clickable peptide nucleic acid-based molecular locks

Brigit Meindl, Agnes Lenz, Hannes Mikula, Brigitte Holzer
Institute of Applied Synthetic Chemistry, TU Wien, Austria

Peptide nucleic acids (PNAs) are synthetic nucleic acid analogues featuring a neutral *N*-(2-aminoethyl)glycine backbone, which enable high-affinity and sequence-selective recognition of complementary RNA.[1] Their ability to selectively bind RNA renders PNAs attractive for potential modulation of disease-relevant RNA targets.[2] While PNAs provide a robust platform for nucleic acid recognition, strategies to achieve persistent and structurally defined RNA binding remain limited.
Here, we present a PNA-based molecular locking approach in which an antisense probe hybridizes to a target RNA and is subsequently interlocked through bioorthogonal click chemistry. We demonstrate the rational design of clickable PNAs and biocompatible locks, exploiting the rapid and selective reaction between 1,2,4,5-tetrazine (Tz) and trans-cyclooctene (TCO) functionalities, resulting in covalent interlocking of the PNA-RNA duplex (Fig.1).
The influence of linker geometry on locking efficiency is investigated using surface plasmon resonance (SPR) spectroscopy. PEG-based linkers of varying length were compared, revealing insights on the geometrically optimal configuration for effective molecular locking of a 10mer PNA-RNA complex and compared to non-locked duplexes. This work establishes molecular locking as a modular, geometry-driven strategy for stabilizing PNA-RNA assemblies.

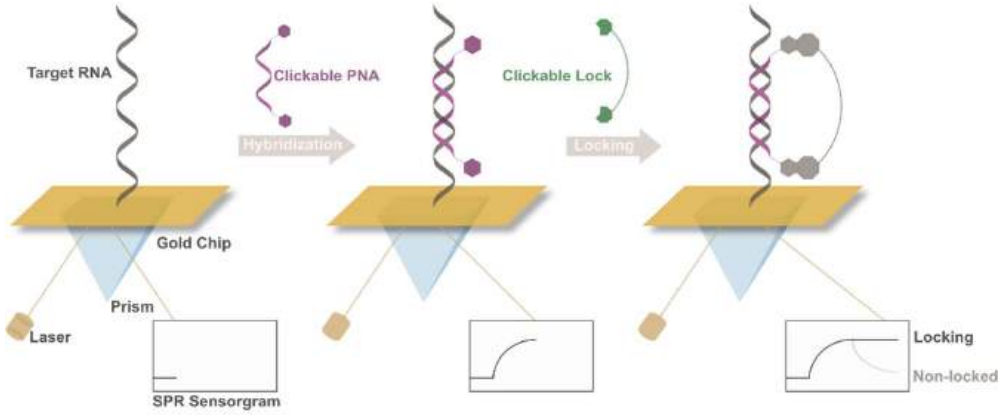

Fig. 2. Bioorthogonal Locking of immobilized target RNA applying a clickable PNA and lock monitored by SPR spectroscopy.

This project was financially supported by the Austrian Science Fund (FWF) (Grant No.10.55776/ZK29).

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CBF - D2 - O09

Bioinorganic hybrid nanoplatforms based on cellulose nanocrystals for mitochondrial damage and cuproptosis induction in tumor cells

Alessia Distefano[1], Marina Scarpa[2], Paolo Bettotti[2], Giovanni Li-Destri[1], Giuseppe Grasso[1], Laura Cifalinò[1], Giulia Annesi[3], Valeria Scalcon[3], Alessia Sambugaro[4], Erik Murador[4], Chiara Nardon[4], and Valentina Oliveri[1]
[1]Dept. Chemical Sciences, University of Catania, Catania, Italy; [2]Dept. Physics, University of Trento, Trento, Italy; [3]Dept. Biomedical Sciences, University of Padova, Padova, Italy; [4]Dept. Biotechnology, University of Verona, Verona, Italy

Cellulose nanocrystals (CNCs) are sustainable nanomaterials well suited for biomedical applications thanks to their nanoscale needle-like morphology, biocompatibility, biodegradability, and easily tunable surface chemistry. These qualities support effective cellular uptake, enhanced tumor accumulation, prolonged circulation, and minimal cytotoxicity. TEMPO-mediated oxidation introduces carboxyl groups, boosting colloidal stability and enabling covalent conjugation. [1]

In parallel, increasing evidence highlights the central role of copper (Cu) in cancer biology. Tumor cells exhibit cuproplasia, a pathological dependence on Cu. Conversely, excess intracellular Cu can cause cuproptosis, a regulated cell death process linked to mitochondrial failure. This dual function makes Cu homeostasis a crucial therapeutic target in cancer, fueling renewed interest in Cu ionophores.[2,3]

In this context, we investigated TEMPO-oxidized CNCs as nanocarriers for Cu ions. CNCs were functionalized with Cu-binding agents (Fig.1). Both pristine and functionalized CNCs were characterized by DLS and ζ-potential, FT-IR, and AFM, confirming successful surface modification and preservation of needle-like morphology. UV–Vis titrations and other experiments demonstrated Cu binding in ligand-functionalized systems, supporting their suitability as Cu nanocarriers.

Biological assays revealed that Cu-loaded functionalized CNCs are active across different cancer cell lines, inducing significant cell death. Mechanistic investigations using complementary techniques indicate mitochondrial damage, consistent with activation of a cuproptotic pathway. These findings suggest that CNC-based Cu delivery systems can effectively shift Cu from a proliferative factor to a cytotoxic trigger in cancer.

This work demonstrates that functionalized CNCs represent a sustainable and tunable inorganic–organic hybrid platform for Cu delivery and induction of cuproptosis, providing new opportunities for designing copper-based nanotherapeutics.

This research received funding from NESTOR (2022BTMYWZ), Menace@CO2.

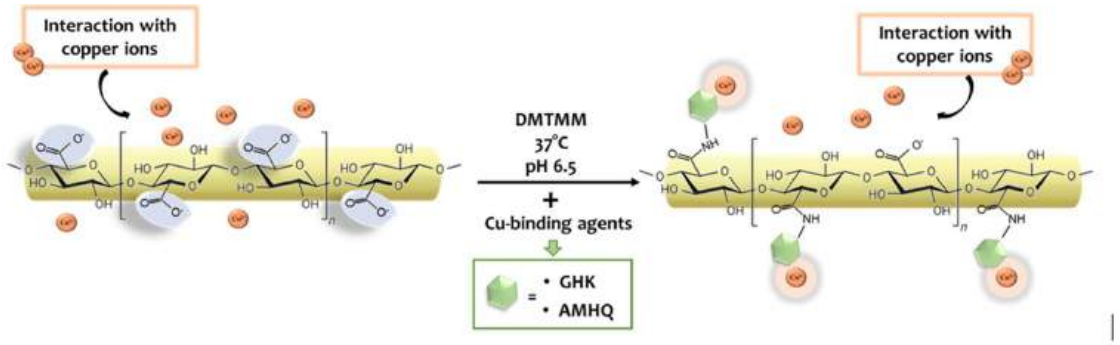

Fig.1 Pristine CNCs (left) and CNCs functionalized with Cu-binding agents (GHK and AMHQ) for Cu delivery (right).

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CBF - D2 - O10
Stimuli responsive biopolymer based nanocarriers for the delivery of hydrophilic cargo

Anitha Ethirajan[1,2]
[1]Hasselt University, Institute for Materials Research (IUMAT), Hasselt, Belgium; [2]imec, IUMAT, Diepenbeek, Belgium

Stimuli responsive nanocarriers (NCs) have continuously gained attention for drug delivery applications. Particularly, NCs based on responsive polymers have gained attention owing to their ability to undergo change in structural conformation/composition under the influence of various physical, chemical and biological stimuli. In complex biological microenvironments, responsive nanocarriers responding to endogenous triggers are of significant interest as payload can be released rapidly and selectively by taking advantage of a unique biochemical environment (e.g., difference between tumor and normal tissues). As redox imbalance (excess reactive oxygen species (ROS) and glutathione (GSH) production) is characteristic of many disease conditions (e.g., tumor, inflammation), NCs designed for cargo release at the target sites that exhibits high ROS/GSH levels has evoked enormous interest.
As dextran and hyaluronic acid (HA) are widely used biopolymers in the development of various drug delivery platforms, in this contribution, our recent work on the ROS and GSH responsive biopolymers based NCs and their potential in cancer therapy will be presented[1,2]. Various hydrophilic cargo containing NCs were successfully synthesized using interfacial polymerization employing the miniemulsion technique and subsequently characterized. The encapsulation efficiencies of the payloads in the NCs were between 80-95%. The release kinetics systematically studied under respective ROS and GSH conditions showed a clear stimulus responsive release trend. Additionally, release was studied using enzymes that can degrade the biopolymers. Biocompatibility and cellular uptake experiments were also carried out. The promising results highlight the huge potential of biopolymer based responsive NCs to deliver hydrophilic therapeutics in complex biological milieu as in tumor.

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CBF - D2 - O11

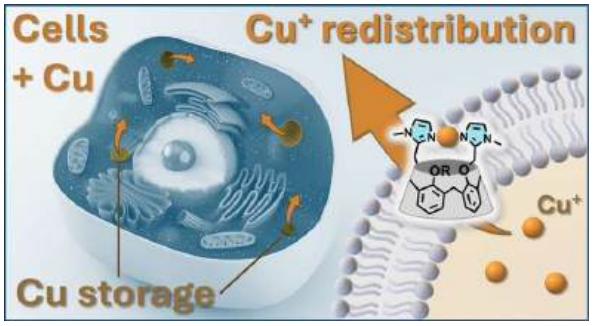
Copper transport across cell membranes by calix[4]arene-based cationophores leading to potent biological activity

Nathan Renier[1], Gianluca Weyckmans Mele[1,2], Pierre Lelièvre[3,4], Mélanie Boeckstaens[5], Anna Maria Marini[5], Lucie Sancey[4], Benoit Busser[4], Giulia Veronesi[3], Ivan Jabin[2], Aurélien Deniaud[3], Hennie Valkenier[1]

[1]Université libre de Bruxelles (ULB), Engineering of Molecular NanoSystems, Brussels, Belgium; [2]Université libre de Bruxelles (ULB), Laboratoire de Chimie Organique, Brussels, Belgium; [3]Univ. Grenoble Alpes (UGA), CNRS, CEA, IRIG, Laboratoire de Chimie et Biologie des Métaux, Grenoble, France; [4]Univ. Grenoble Alpes (UGA), INSERM U1209, CNRS UMR 5309, Institute for Advanced Biosciences, Grenoble, France; [5]Université libre de Bruxelles (ULB), Biology of Membrane Transport Laboratory, Gosselies, Belgium

Lipid bilayers are impermeable to ions, including copper cations. Copper is an essential trace element for life, present in the active site of various enzymes, whereas free copper is detrimental inside cells. Copper homeostasis is thus finely controlled, involving Cu(I) transporting membrane proteins Ctr1 and ATP7A/B. Disruption of copper homeostasis has been reported as a potential anti-cancer strategy.

With this objective, we have developed a series of lipophilic compounds with two copper coordinating (benz)imidazole groups that are able to function as ionophores, transporting copper cations across membranes.[1,2] This was firstly demonstrated in liposomes with a Cu(I) sensitive fluorescent probe encapsulated.[1] Secondly, Cu transport across cell membranes was studied in yeast cells with Ctr1 deleted. This deletion shuts down their respiration pathway, as one of the proteins involved requires Cu in its active site. Addition of our Cu ionophores resulted in the restoration of yeast growth. Thirdly, cytotoxicity studies in hepatocarcinoma cells highlighted the crucial role of the lipophilicity of Cu ionophores for their activity in cells. Further studies on one of the most potent compounds (Cuphoralix) showed that Cu ionophores cause a redistribution of the intracellular Cu from vesicles to the cytosol.[2]



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CBF - D2 - O12
Glycosylated mycotoxins in food: A hidden enemy

Vladimír Křen[1], Jitka Brouzdová[1,2], Adam Behner[2], Milena Stránská[2]
[1]Institute of Microbiology of the Czech Academy of Sciences, Czech Republic; [2]University of Chemistry and Technology in Prague, Czech Republic

Mycotoxins are toxic secondary metabolites produced by filamentous fungi and represent a persistent challenge to global food safety. Beyond well-known free mycotoxins, recent research has highlighted “masked” mycotoxins - glycosylated derivatives formed mainly by plants through enzymatic conjugation as part of their detoxification response. These compounds often escape routine analytical detection, remain stable during food processing, and can be hydrolyzed back to their toxic parent compounds during digestion, complicating exposure assessment and risk management.[1]
This presentation addresses the occurrence, formation, and toxicological relevance of glycosylated derivatives of major mycotoxins, including trichothecenes (deoxynivalenol, T-2, HT-2), zearalenone (ZEN), ochratoxins, *Alternaria* toxins, and ergot alkaloids in cereals and plant-derived foods. Glycosylation is primarily catalyzed by plant UDP-glucosyltransferases (UGTs), producing conjugates such as DON-3-glucoside and ZEN-14-glucoside. Microorganisms, including yeasts and detoxifying fungi, also contribute to these transformations. Chemically synthesized glycosides have been instrumental in establishing analytical standards and elucidating stereochemistry and biological activity. Although masked mycotoxins generally show reduced acute toxicity *in vitro*, their persistence during thermal processing and enzymatic cleavage in the gastrointestinal tract raise concerns about delayed exposure. For example, DON-3-glucoside and T-2-3-glucoside can survive extrusion and be hydrolyzed by gut microbiota, releasing the parent toxins. ZEN glucosides may likewise regenerate estrogenic metabolites *in vivo*.
Detection of modified mycotoxins is an emerging priority. LC-MS/MS methods increasingly include glycosides, and enzymatic hydrolysis is used to estimate total toxin burdens. However, limited availability of standards and toxicological data hampers regulation. Given their widespread occurrence and biological reactivation, glycosylated mycotoxins represent a critical frontier in ensuring food safety.

Supported by Czech Science Foundation project 24-10000S and project Talking microbes-understanding microbial interactions within One Health framework (CZ.02.01.01/00/ 22_008/0004597) from the Ministry of Education, Youth and Sports of the Czech Republic.

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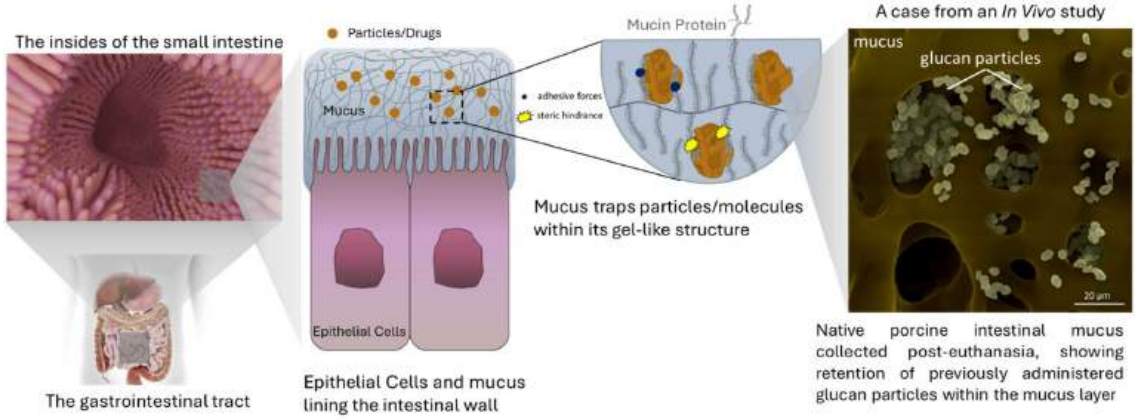
CBF - D2 - O13
Development of a biosimilar mucus layer as a predictive tool for preclinical drug assessment

Suada Đukaj[1], Denisa Lizonová[1], Josef Beránek[2], František Štěpánek
[1]*University of Chemistry and Technology Prague, Czechia;* [2]*Zentiva s.r.o., Czechia*

The mucus layer is a viscoelastic hydrogel that overlays the intestinal epithelium, serving as a protective barrier against microorganisms while simultaneously affecting drug absorption *(1)*. Many orally administered drugs exhibit poor bioavailability, thus failing to reach the epithelium (Fig. **1**), as mucus impedes their molecular transport *(2)*. Reliable extrapolation to *in vivo* drug transport requires physiologically relevant *in vitro* models that reproduce native mucus's composition, microstructure, and rheology. Cell-based systems, such as HT-29 MTX cells, secrete mucus, but produce variable amounts with poorly characterized viscoelastic properties *(3)*. To address these limitations, we developed a biosimilar mucus that recapitulates the structural, compositional, and rheological characteristics of native mucus and can be prepared in-house. The biosimilar mucus formulation is based on laboratory-extracted mucins (

Fig. **2**) i.e. the main proteins found in mucus, that retain environmental responsiveness, particularly to pH and divalent cations such as Ca^{2+}, unlike common commercial mucins, which are functionally impaired *(4)*. By combining the laboratory-extracted mucins with selected mucus components, we successfully reproduced critical rheological parameters, including viscosity, storage, and loss modulus, through direct benchmarking against native mucus. Surface chemistry was likewise validated, as the biosimilar model closely matched the zeta potential of native mucus. To establish an *in vitro* model that accurately mimics intestinal mucus thickness, we employed 3D bioprinting to generate a homogeneous mucus layer of defined thickness within a Trans-well system. We then conducted permeation studies using FITC-DEXTRAN molecules of varying sizes, demonstrating that its permeability closely matches that observed in native mucus. Moreover, the model exhibited cell compatibility with Caco-2 cells, supporting its successful integration into epithelial transport studies. Collectively, the cell-compatible biosimilar mucus provides a



predictive tool for early-stage drug preclinical assessment, guiding rational drug redesign to improve passage

Fig. 1. Intestinal mucus traps particles and molecules, limiting their diffusion to the epithelium and thereby reducing drug bioavailability

through this biological barrier and reduce late-stage project failures in the pharmaceutical industry.

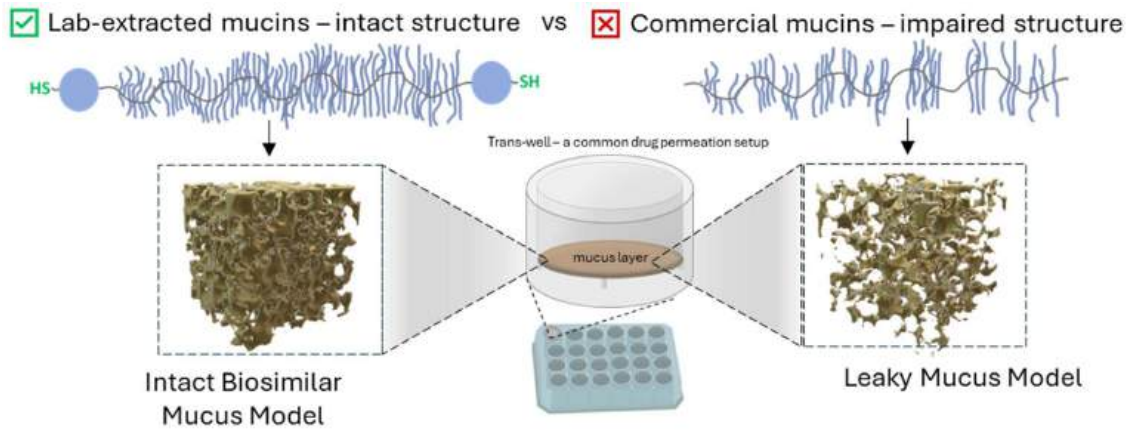


Fig. 2. Concept of the biosimilar mucus layer: a trans-well setup portraying intact biosimilar mucus prepared from laboratory-extracted mucins that retain native functionality, unlike commercially available mucins with impaired structure that overestimate drug permeation.

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CBF - D2 - O14

A coarse-grained approach to modelling adsorption of the lubricating salivary protein, MUC5B, to biomimetic tongue surfaces

Thilakan Kanesalingam[1], Erik Weiand[1], Philippa M. Cann[1], Marc Masen[1], James P. Ewen[1,2]
[1]Imperial College London, UK; [2] University of Bath, UK

Saliva plays a crucial role in the lubrication of oral surfaces, aiding the swallowing of foods. Central to its lubricating properties is the mucin glycoprotein, MUC5B, containing several negatively charged glycans, which are readily solvated by water and confers excellent hydration lubrication[1]. The mechanism underlying the adsorption of MUC5B to oral surfaces has yet to be fully resolved and can effectively be addressed through nanoscale insights from molecular dynamics (MD) simulations. Here, we aim to characterise the free energy landscape of MUC5B's adsorption using a coarse-grained MD model of a biomimetic tongue surface and MUC5B within the MARTINI 3 framework. Screening of biomimetic polymers via contact angle analysis of water droplets modelled on polymers reveals Polycaprolactone (PCL) and Nylon 6,6 (PA66) as suitable models of the tongue's surface with comparable wetting properties. To support our study, we also develop a coarse-grained model of MUC5B[2], comprising of a short glycopeptide joined to a cysteine domain of MUC5B. We parameterise new MARTINI 3 bond terms for mucin glycans from all-atom simulations (CHARMM36m), with the conformation of the model's glycosylated domain closely aligning to experiments, as determined by Flory's exponent. Subsequently, extended adaptive biasing force simulations are employed to map the free energy landscape of MUC5B's adsorption to PCL and PA66 using the potential of mean force, illustrating MUC5B's adsorption to be driven by its cysteine domain. Alongside future adsorption simulations exploring the contributions of individual amino acids, we anticipate our findings will provide deeper insight into saliva's lubricating mechanism, aiding the development of saliva substitute therapies.

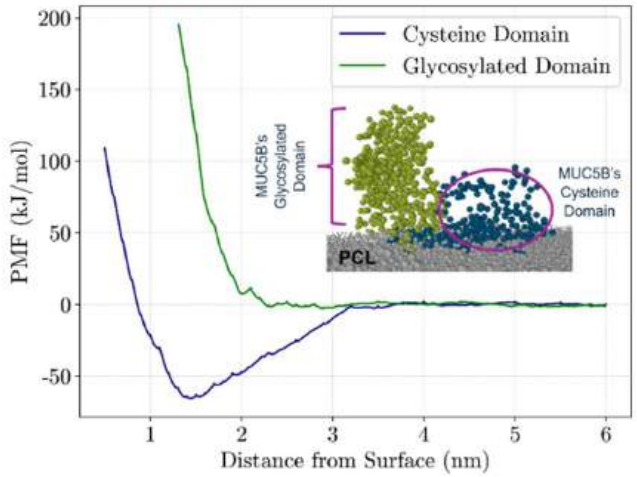

Fig. 1. Potential of Mean Force (PMF) as a function of the distance between Polycaprolactone (PCL) and MUC5B's cysteine (blue) and glycosylated (green) domain.

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CBF - D2 - O15
From femtoseconds to seconds: Time-resolved crystallography of photolyases and cryptochromes

Manuel Maestre-Reyna[1,2]
[1]Dept. of Chemistry, National Taiwan University; Taiwan; [2]Institute of Biological Chemistry, Academia Sinica; Taiwan

Protein function encompasses very different time-scales, spanning from chemical reactivity in femto- to picoseconds to conformational changes that take place in milliseconds or beyond. In most cases, the biological systems that proteins interface with are even slower. For example, upon light-absorption, cryptochrome photoreceptors undergo a virtually instantaneous electronic transition of their oxidized flavin chromophore, which is relaxed over hundreds of femtoseconds by chromophore single electron reduction paired with protein oxidation [1] (Fig. 1A). The resulting radical pair evolves over several hundreds of picoseconds, ultimately leading to partial protein unfolding (Fig.1B) in the sub-second range, which reveals new potential interaction surfaces for signaling [2-3]. Accordingly, a fundamental property of protein dynamics generally, and cryptochrome activity in particular, must be to exert exceptional timing control to ensure that ultrafast events consistently trigger much slower responses. In recent years, time-resolved crystallography (TRX) at X-ray Free Electron Lasers (XFEL) has revolutionized the field of protein dynamics, ensuing in an age of protein cinematography [4]. By adapting these techniques first established at XFELs to study ultrafast events to synchrotron X-ray sources [5], we have gained access to slower time domains. In my talk, I will discuss how we made use of three different TRX setups to follow how light-driven ultrafast electron transfer in a cryptochrome photoreceptor in femtoseconds can trigger a large-scale order-disorder phase transition in seconds, revealing the molecular basis for the elegant dance of the protein across vastly different time-scales.and affiliations.

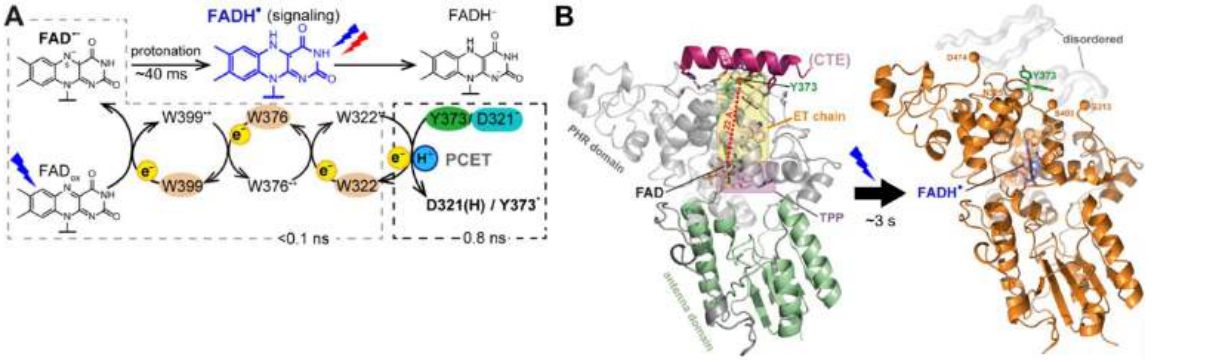

Fig. 1. Light-driven reactivity of an animal-like cryptochrome. (A) Flavin Adenine Dinucleotide (FAD) chromophore redox reactivity and kinetics. (B) Dark- and light-adapted cryptochrome structures obtained by serial femtosecond crystallography.

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CBF - D2 - O16
Design of semiconducting polymer interfaces to control Schwann cell behaviour

Stefania Gardoni[1], Tianyang Liu[1], Chao Lyu[1], Robert Malinowski[1], Matthew Blunt[1], Megan Westwood[2], James B. Phillips[1], Bob C. Schroeder[1]
[1]University College London, UK; [2]Chalmers University of Technology, Sweden

Understanding how cell behaviour is regulated by interactions with external surfaces is central to scaffold design and tissue engineering for nerve regeneration and wound repair. Cell adhesion and differentiation depend on surface morphology, topography, wettability and surface energy, which determine protein adsorption at the biointerface and cytoskeleton organisation[1]. Semiconducting polymers have emerged as promising bioelectronic and tissue-interface materials because they are processable, can be engineered to be biocompatible, and offer rich opportunities for chemical functionalisation and nanoscale morphology control, enabling systematic tuning of interfacial and electronic properties[2]. In this work, three isoindigo-based semiconducting polymers (g-pIID-T, a-pIID-T and f-pIID-T) with a common conjugated backbone and side chains of identical length but different polarity and hydrophobicity were designed to tune thin-film surface properties for Schwann cells, the glial cells responsible for myelination and support in the peripheral nervous system. Quantitative surface characterisation showed that the three polymers span a wide, well-defined range of wettability, with water contact angles from ≈25° to ≈102°, accompanied by distinct nanoscale morphologies, from more cratered, nanohole-rich surfaces to smoother, wave-like films within a single isoindigo-based platform. Schwann-cell assays established clear correlations between these surface properties and cell behaviour. On g-pIID-T, cells adhere but remain relatively rounded; on a-pIID-T, they adopt elongated, well-spread morphologies with higher coverage; on f-pIID-T, cells are less spread and preferentially occupy more favourable regions of the surface. Together, these results show that simple side-chain changes on an isoindigo backbone can tune neural cell adhesion and morphology in a predictable and reproducible way, providing practical design rules for semiconducting polymer interfaces relevant to peripheral nerve repair and the broader engineering of bioelectronic materials with targeted cellular responses.

This work was supported by the UK EPSRC grant EP/S023054/ and UKRI Future Leaders Fellowship MR/Y003802/1.

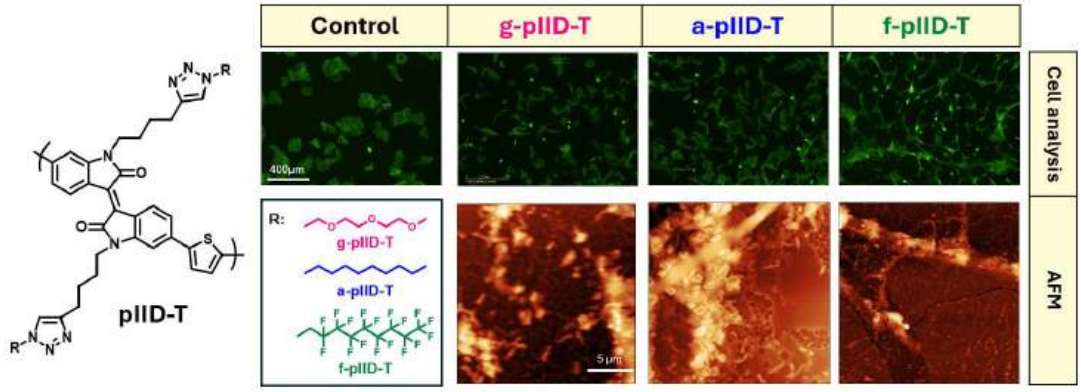

Figure 1. (Left) Chemical structures of g-pIID-T, a-pIID-T, and f-pIID-T copolymers, and (right) optical microscope and AFM height images of Schwann cells seeded on the corresponding polymer films. Schwann cells were fixed and stained with phalloidin and imaged in the IncuCyte system using the green fluorescence channel after 48 h of incubation on the three polymer surfaces.

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CBF - D2 - O17

Uncovering phospholipid and oxysterol signatures in pancreatic ductal adenocarcinoma cells and their extracellular vesicles

Cosima Damiana Calvano[1,2], Vito Nettis[1], Giovanni Ventura[1,2,] Andrea Castellaneta[1], Liam McDonnell[3], Noa Ndimurwanko[3], Tommaso Cataldi[1,2]

[1]Dipto di Chimica, [2]Centro interdipartimentale SMART, Università degli Studi di Bari Aldo Moro, Italy; [3]Fondazione Pisana per la Scienza, Via Ferruccio Giovannini, Italy

Pancreatic ductal adenocarcinoma (PDAC) is one of the most aggressive and lethal cancers with an extremely poor prognosis (five-year survival rate of 7%) due to the high heterogeneity of tumours, late diagnosis, and high resistance to chemotherapies. Typically, blood tests such as carbohydrate antigen (CA) 19-9, either alone or in combination with other blood proteins, are considered for PDAC screening[1]. Magnetic resonance imaging, computed tomography, endoscopic ultrasound, and positron emission tomography remain the most reliable tools for PC diagnosis in clinical practice. Circulating tumour DNA and extracellular vesicles (EVs) as exosomes (30–150 nm), microvesicles (50-1000 nm), and apoptotic bodies (≥500 nm) are emerging as promising tools for the early diagnosis of PDAC[2]. This study focuses on the comprehensive analysis of phospholipid (PL) and oxysterol in terms of composition and concentration in cells and Evs from healthy (HPNE) and cancer cells (PANC1) grown under normoxic and hypoxic conditions. The research aims to identify novel circulating biomarkers for early PDAC detection, addressing the limitations of current diagnostic approaches and ultimately improving prognostic accuracy and therapeutic outcomes. Lipid extraction was performed after a total exosome isolation from healthy and cancerous cells, collected and filtered through 100kDa MWCO filters. Hydrophilic interaction liquid chromatography (HILIC) and reversed-phase LC coupled with electrospray ionization high-resolution Fourier-transform mass spectrometry (ESI FTMS) were employed to analyze phospholipid and oxysterol profiles, respectively. The study employed a metabolomics approach[3] with integrated quality control (QC) samples for PL to ensure analytical consistency, while oxysterols were quantified using authentic standards. In both signatures, preliminary interesting outcomes on discriminant lipid species were retrieved. Further, the profiles of the corresponding HPNE and PANC1 EVs revealed significant differences.

Acknowledgments: This work is supported by “Fondo per la Qualità e l’Internazionalizzazione della Ricerca” (issued by D.R. No. 2924 on 29/07/2024), financed by the University of Bari Aldo Moro.

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CBF - D2 - O18

Functional characterization of mitochondrial 3-ketoacyl-CoA thiolase (*kat-1*) in *C. elegans* using comparative metabolomics

Marie-Désirée Schlemper-Scheidt, Siva Bandi, Stephan H. von Reuss
University of Neuchâtel, Switzerland

Mutation of mitochondrial 3-ketoacyl-CoA thiolase (*kat-1*) shortens *C. elegans* lifespan but its function remains enigmatic.[1]

Comparative metabolomics of *C. elegans* wild-type (N2) and *kat-1(tm1037)* highlighted *kat-1* enriched compounds. Their NMR characterization revealed modular glucosides (MOGLs), with tigloyl as common feature. Incorporation experiments utilizing an *E. coli Δile Δleu Δval* mutant as food source that could be specifically enriched with either L-[U-$^{13}C_5$]-valine, L-[U-$^{13}C_5$,^{15}N]-leucine, or L-[U-$^{13}C_5$,^{15}N]-isoleucine highlighted metabolites derived from branched chain amino acid metabolism. Tigloyl units of the *kat-1* enriched MOGLs were [$^{13}C_5$]-enriched upon incorporation of or L-[U-$^{13}C_5$,^{15}N]-Ile, identifying it as 2-methylacetoacetyl-SCoA thiolase in mitochondrial L-isoleucine metabolism. Free *anteiso*-C5 acids upstream of 2-methylacetoacetic acid were also [$^{13}C_5$]-labelled upon incorporation of L-[U-$^{13}C_5$,^{15}N]-Ile and enriched in *kat-1*. Increased flux of *anteiso*-C5 building blocks from mitochondria characterized by ESI-(+)-MS^E screening for *O*-acyl carnitines demonstrated that *O*-C5-L-carnitines are strongly enriched in *kat-1*. Furthermore, mutations in *glo-1(zu391)*, *glo-3(kx94)*, and *glo-4(ok623)*, essential for lysosome-related organelle formation, demonstrated suppression of tigloyl-substituted MOGL formation.[2,3]

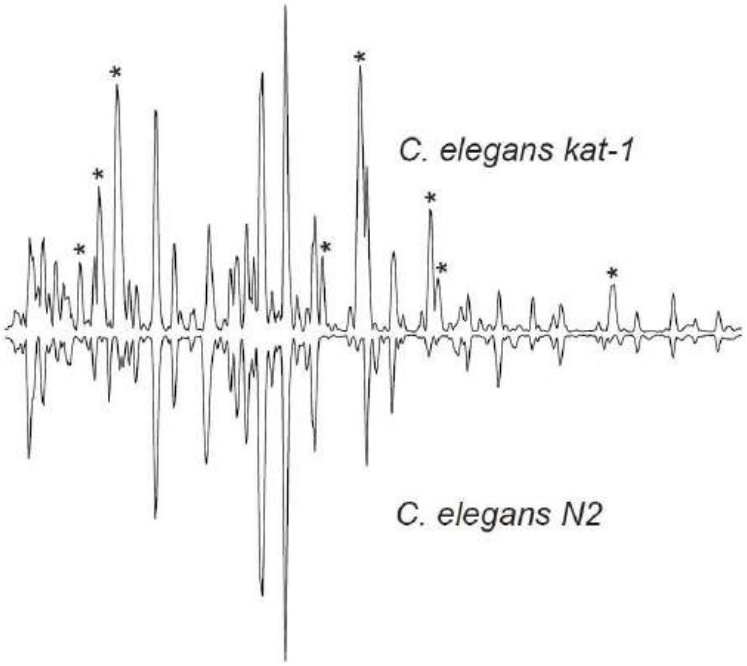

Fig. 1. Comparative metabolomics of exometabolomes of a *kat-1* mutant (above) and a *N2* control (below). The markers indicate some of the metabolic changes found in the HPLC-MS exometabolome traces.

Our results provide a functional characterization of *kat-1* as mitochondrial 2-methylacetoacetyl-SCoA thiolase and demonstrates that mitochondrial L-isoleucine metabolism provides tigloyl building blocks, exported via the carnitine shuttle and utilized for the biosynthesis of MOGLs in lysosome-related organelles. How this pathway results in lifespan reduction of *kat-1(tm1037)* remains to be identified. Consequently, *C. elegans kat-1* represents a potential model system for mitochondrial acetoacetyl-CoA thiolase (T2) deficiency, a rare human disease.[4]

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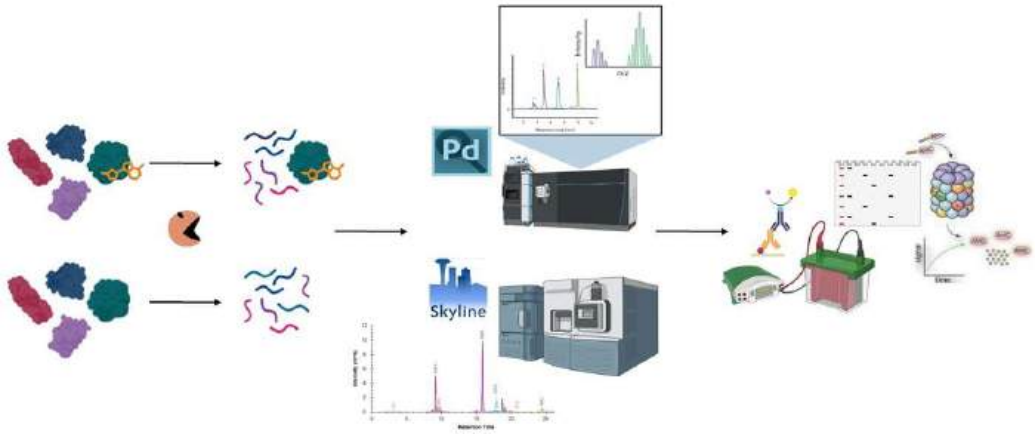
CBF - D2 - O19
Functional proteomics-driven discovery of quinazolinones as proteasome inhibitors

Elva Morretta[1], Claudia Finamore[1], Simona De Marino[1], Elisabetta Panza[1], Matteo Mozzicafreddo[2], Angela Zampella[1], Carmen Festa[1], Maria Chiara Monti[1]
[1]Dept. of Pharmacy, University of Naples "Federico II", Naples, Italy; [2]Dept. of Clinical and Molecular Sciences, Marche Polytechnic University, Ancona, Italy

Quinazolinones are privileged scaffolds in drug discovery, being characterized by chemical stability, synthetic accessibility, and a broad biological activities spectrum, including antihypertensive, anticancer, and antiviral ones[1]. In this scenario, we investigated the bioactivity of a focused set of 4-(3H)-quinazolinone derivatives. Initially, compounds' cell permeability was assessed through parallel artificial membrane permeability assay, followed by an evaluation of their cytotoxicity in breast (MDA-MB-231 and MCF-7) and prostate (DU-145) cancer cells. This screening identified compound 4k as the most cytotoxic molecule and DU-145 as the most responsive cellular model.
To elucidate the molecular basis of compound 4k–induced cytotoxicity, we characterized its interactome in DU-145 lysates using label-free and limited-proteolysis–based functional proteomics approaches. These methodologies enable in-solution investigation of protein–small molecule interactions by monitoring ligand-induced conformational changes at either the protein or peptide level. Accordingly, our strategy combined the protein-centred Drug Affinity Responsive Target Stability (DARTS)[2] and the peptide-centred targeted Limited Proteolysis coupled to Multiple Reaction Monitoring mass spectrometry (t-LiP-MRM)[3] strategies. DARTS served the purpose of identifying proteins with altered proteolytic susceptibility upon binding to compound 4k, while t-LiP-MRM enabled mapping of ligand-induced conformational changes, thereby pinpointing protein regions directly or allosterically involved in the binding process.
DARTS analysis revealed several subunits of the 26S proteasome as the most reliable compound 4k biological targets. Among them, t-LiP-MRM confirmed that the proteasomal β2 and β5 subunits were affected at the peptide level, as further supported by molecular docking. Then, functional assays demonstrated compound 4k ability to both inhibit proteasomal chymotrypsin- and trypsin-like activities in vitro and induce accumulation of polyubiquitinated proteins in DU-145 cells, confirming proteasome inhibition as a key mechanism underlying this molecule's cytotoxic activity.



Schematic representation of the functional proteomics-based target deconvolution strategy. DARTS (upper panel) and t-LiP-MRM (lower panel) identified β2 and β5 proteasomal subunits as compound 4k partners, confirmed by in vitro and in cell assays.

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[3]Feng, Y.; *et al. Nat. Biotecnol.* **2014**, *32*, 1036-1044.

CBF - D2 - F01
Quinoline based luminescent imidazolium salts as vector for gene therapy

Justine Kapp[1], Laurent Douce[2]
[1]University of Strasbourg, France; [2]Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, France

Molecular salts, particularly those based on imidazolium units, have attracted the attention of the scientific community due to their unique properties and structural versatility, especially those containing a fluorophore[1,2]. Indeed, light and the phenomena associated with it, such as fluorescence, have proven to be a powerful and highly sensitive tools for exploring the nanoscale world. Cationic lipids have, for several years, emerged as the best candidates for the delivery of genetic material and thus for gene therapy[3]. In 2009, *Dobbs et al*, demonstrated that the delivery of siRNA was possible using imidazolium salts. In this context, we have designed new imidazolium salts incorporating a quinoline unit to create a novel theragnostic agent. Owing to its lone pair bearing nitrogen atom, quinoline is capable of interacting with protons and is therefore an ionizable unit. Our molecular design combines three components: a rigid hydrophobic fluorophore, a rigid hydrophilic imidazolium core, and flexible hydrophobic alkyl chains. The combination of these three antagonist parts makes these salts a new type of highly bioavailable and luminescent molecular platform. This structural arrangement allows for fine-tuning of both the amphipathic and amphiphilic character of our salts, thereby enabling control over the emergence of their biological properties and mesomorphic properties. The quinoline ring offers seven different substitution positions, allowing the establishment of a structure–activity relationship and the supramolecular level study of the behavior of these molecules. Herein, we will present the synthesis and the study of the biological properties of these salts as a function of their substitution position on the quinoline unit.

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Graphical abstract:

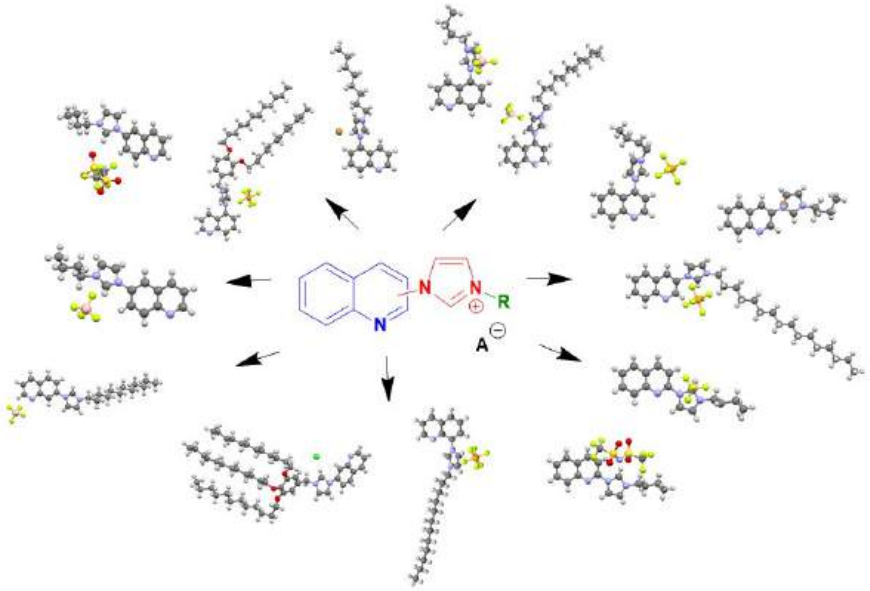

Fig. 1. Schematic representation of our imidazolium with the three antagonist parts (blue: rigid and hydrophobic, red: rigid and hydrophilic, green: flexible and hydrophobic) and X-ray structure of some synthesized compounds.

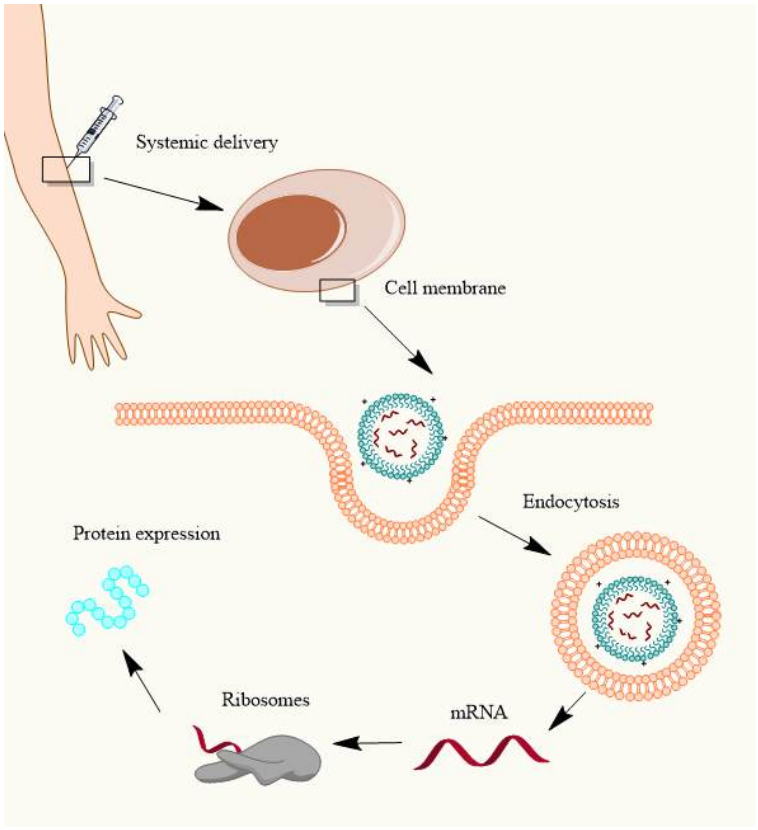

Fig. 2. Schematic representation of the transfection process: systemic delivery of the drug, lipoplexe interactions with cell membrane, endocytosis, endosomal escape, translation of mRNA, protein expression of the transfected gene.

CBF - D2 - F02
Designing antibacterial materials using cysteine

Oana Grad, Anzar Khan
National Institute for Research and Development of Isotopic and Molecular Technologies, Romania

Cysteine is the only natural amino acid that contains a thiol group, which can participate in disulfide bond formation and bind with metal atoms. As a result, cysteine plays a vital role in stabilizing protein structures and facilitating enzymatic reactions that require a metal cofactor. Because of these properties, cysteine is an appealing building block for material synthesis. We hypothesized that the sulfur atom in cysteine could be converted into a sulfonium cation through a series of alkylation reactions. This conversion might allow the creation of cysteine-based electrolytes with alkyl chains that penetrate membranes, a zwitterionic structure to enhance compatibility with mammalian cells, and a sulfonium cation capable of disrupting bacterial cell membranes via electrostatic interactions. To test our hypothesis, we began developing an efficient synthetic route to produce the desired materials. The first step involved using thiol-epoxy "click" chemistry with various epoxide substrates. This reaction, conducted in water, successfully converted the starting materials into the targeted thioethers. We are currently working on transforming these thioethers into sulfonium salts. In this work, we will focus on discussing the synthetic feasibility of producing cysteine-based cationic antibacterial materials, which could potentially be converted into antibacterial sulfonium salts through alkylation of the sulfur atom.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CNCS - UEFISCDI, project number PN-IV-P1-PCE-2023-0441, within PNCDI IV.

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CBF - D2 - F04

Biomimetic aqueous-core hydrogel microcapsules for spatially organized enzymatic cascade reactions

Chae-Hee Park[1], Tae Jung Park[2], Jong Pil Park[3], Changyeon Lee[4], Hyunmin Yi[5], Chang-Hyung Choi[1]
*[1]*School of Chemical Engineering, Yeungnam University, *Republic of Korea; [2]Dept. of Chemistry,* Chung-Ang University, *Republic of Korea; [3]Dept. of Food Science and Technology, Chung-Ang University, Republic of Korea; [4]Dept. of Chemical Engineering, Chung-Ang University, Republic of Korea; [5]Dept. of Chemical and Biological Engineering, Tufts University, USA*

Enzymatic cascade reactions are widely used in biosensing, biocatalysis, and therapeutic applications, yet their performance is often limited by enzyme incompatibility, molecular crowding, and inefficient mass transfer in homogeneous systems. Inspired by the compartmentalized organization of eukaryotic cells, this work presents a microfluidic strategy for constructing aqueous-core hydrogel microcapsules that enable spatially organized enzymatic cascades. Using droplet-based microfluidics, triple-emulsion templates are generated and converted into core–shell hydrogel microcapsules, allowing selective localization of different enzymes in distinct compartments, exemplified by glucose oxidase confined within the aqueous core and horseradish peroxidase incorporated into the surrounding hydrogel shell. High encapsulation efficiency is achieved while preserving enzyme activity, and spatial separation of enzymes is designed to facilitate substrate diffusion and reduce unfavorable interactions, thereby providing a controlled microenvironment for cascade reactions. Key structural features, including the core-to-shell volume ratio and core position, are readily tunable through microfluidic control, while the hydrogel shell properties can be adjusted to regulate molecular permeability and enzyme retention, offering flexibility for different reaction schemes and operating conditions. Overall, this biomimetic microcapsule platform provides a versatile approach for organizing enzymatic cascades within confined microenvironments and holds promise for applications in biosensors, artificial microreactors, and advanced delivery systems, with ongoing work focused on quantitative performance evaluation and extension to more complex multi-enzyme networks.

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2025-02233102)

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CBF - D2 - F05

Design and synthesis of novel sugar-based antibacterial agents against Gram-negative bacteria

Catarina Maria[1], Nuno M. Xavier[2], Rodrigo F. M. de Almeida[1], Amélia P. Rauter[1]
[1]Centro de Química Estrutural, Institute of Molecular Sciences (CQE-IMS), Faculdade de Ciências, Universidade de Lisboa, Portugal; [2]Research Institute for Medicines (iMed.ULisboa), Faculdade de Farmácia, Universidade de Lisboa, Portugal

Antimicrobial resistance is recognized by the World Health Organization as one of the top ten health threats. Bacterial resistance is particularly concerning, with Gram-negative bacteria (GNB) being considered as top priority by the same organization. GNB are especially challenging due to their intrinsic resistance mechanisms that arise from their complex cell envelope consisting of an inner membrane (IM), a peptidoglycan (PG) cell wall and an outer membrane (OM).[1] Over the past decades, our group has focused on the development of carbohydrate-based antibacterial agents, namely dodecyl deoxyglycosides with activity against Gram-positive bacteria (GPB).[2-5] These compounds act by disrupting the cytoplasmic membrane through interaction with phosphatidylethanolamine (PE) lipids. In GNB, these compounds displayed potential to target the IM through a similar mechanism; however, they were not able to cross the OM.[5] In this context, the present work aims to modify the previously synthesized compounds to target GNB. The PG cell wall of GNB is composed of *N*-acetyl muramic acid-β-1,4-*N*-aceylglucosamine (MurNAc-GlcNAc, Figure 1) repeat units. Based on this structure, we propose the synthesis of carrier-linked prodrugs that mimic this repeat unit. Analogues will be synthesized by coupling a MurNAc moiety to dodecyl deoxyglycosides through a β-1,4 bond. Also, computational studies will be conducted to guide the selection of deoxygenation patterns and molecular structures. Through this approach, we aim to contribute with novel strategies to overcome Gram-negative bacterial resistance.

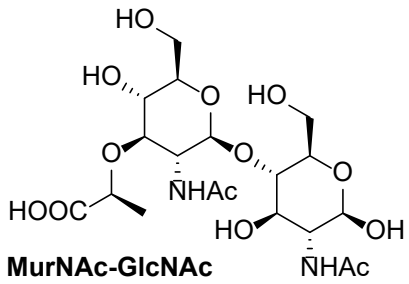

Fig. 1. Structure of the MurNAc-GlcNAc repeat unit.

Acknowledgements: Fundação para a Ciência e a Tecnologia (FCT) is gratefully acknowledged for the granting of the PhD Studentship 2023. 01083. UIDB. Also, FCT is acknowledged for funding of CQE (UID/100/2025) and IMS (LA/P/0056/2020) and iMed.ULisboa (UID/04138/2025).

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CBF - D2 - F08
Cannabizetol: Discovery of a new cannabinoid

Luca Pozzi[1], Andrea Gotti[2], Marco Fumagalli[3], Andrea Citarella[1], Valerio Fasano[1], Giuseppe Paladino[4], Umberto Ciriello[4], Salvatore Princiotto[2], Francesca Annunziata[2], Giulia Martinelli[3], Enrico Sangiovanni[3], Andrea Pinto[2], Mario Dell'Agli[3], Daniele Passarella[1]
[1]Dept .of Chemistry, Università degli Studi di Milano, Milan, Italy; [2]Dept. of Food, Environmental and Nutritional Sciences (DeFENS), Università degli Studi di Milano, Milan, Italy; [3]Dept. of Pharmacological and Biomolecular Sciences "Rodolfo Paoletti", Università degli Studi di Milano, Milan, Italy; [4]LINNEA SA, Riazzino (TI), Switzerland

Phytocannabinoids are a family of more than 150 natural products isolated from *Cannabis sativa L.* extracts.[1] While the biological activity of the four "major cannabinoids" (Δ^9-THC, CBD, CBG, and CBC) has been extensively investigated, information on the "minor cannabinoids" is still limited, mainly due to their presence in trace amounts in plant extracts.[2] Recent efforts have led to the identification of two new cannabinoids characterized by a particular methylene-bridged homodimeric structure: cannabisol[3] and cannabitwinol (CBDD),[4] the homodimers of Δ^9-THC and CBD respectively. In this work[5] we report the discovery of the third member of this rare class of cannabinoids, cannabizetol (CBGD), the homodimer of CBG (Figure 1). The availability of a chemically synthesized standard was crucial for its unequivocal identification, thus confirming the natural occurrence of this new compound. In addition, the skin anti-inflammatory activity of cannabizetol was evaluated in HaCaT keratinocytes, demonstrating a remarkable inhibitory effect on NF-κB signaling and IL-8 secretion. These results highlight cannabizetol as a promising bioactive metabolite with potential dermatological applications. Motivated by these results, we developed a synthetic strategy based on continuous flow chemistry technology, achieving a substantial reduction in reaction times.

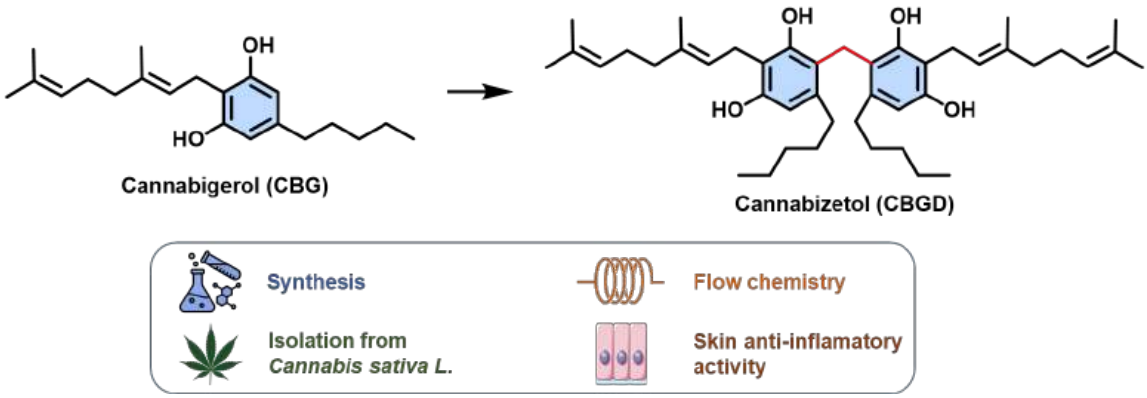

Fig. 1. Chemical structure of cannabigerol (CBG) and cannabizetol (CBGD).

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CBF – D2 – F09

The effect of processing technology on the content of acrylamide, amino acids, and reactive dicarbonyl compounds formed during bread baking

Małgorzata Starowicz[1], Joanna Honke[1], Kristína Kukurová[2], Maria Kopuncova[2], Zuzana Ciesarová[2], Małgorzata Wronkowska[1]

[1]InLife Institute of Animal Reproduction and Food Research, Poland; [2]NPPC, Slovakia

Thermal processing and long-term storage of food initiate complex chemical reactions between carbonyl groups of reducing sugars and amino groups of amino acids, peptides, and proteins. This set of reactions, known as the Maillard reaction, is responsible for desirable flavor, aroma, and color formation, but also for the generation of potentially harmful compounds such as acrylamide and reactive dicarbonyls, including methylglyoxal (MGO) and glyoxal (GO). Free asparagine is recognized as a key precursor in acrylamide formation, and its concentration in cereal raw materials may significantly influence acrylamide levels in processed foods.

The present study aimed to evaluate the content of amino acids and Maillard reaction products in model bakery products obtained from two oat varieties (spring and winter) and to determine the effect of baking parameters on their formation. Breads were prepared under two baking conditions (200°C/90 min and 180°C/120 min). The content of amino acids (Asn, Asp, Gln, Glu), acrylamide, and reactive dicarbonyls (MGO, GO) was determined using previously developed HPLC and LC-MS methods.

Spring oat grain contained approximately twice the level of the analyzed amino acids compared to winter oat; however, this difference was not reflected in the final bread products. Baking parameters significantly affected acrylamide and carbonyl compound formation. Lower temperature combined with extended baking time reduced their levels, whereas increasing temperature and time resulted in a twofold rise in acrylamide content and a fourfold increase after parameter modification in breads from both oat varieties. No significant varietal effect on the analyzed compounds was observed.

The results confirm that time and temperature are critical determinants of Maillard reaction product formation in fresh bread, while further characterization of oat varieties may support the development of improved cereal-based products.

Acknowledgments: This contribution was supported by COST Action CA21149 (Reducing acrylamide exposure of consumers by a cereals supply-chain approach targeting asparagine (ACRYRED); https://acryred.eu/)

CBF - D3 - O01
Protein-G-quadruplex interactions: Expanding frontiers in drug development

Jussara Amato
Dept. of Pharmacy, University of Naples Federico II, Italy

G-quadruplexes (G4s) are non-canonical nucleic acid secondary structures that form in guanine-rich regions of DNA and RNA. Once considered structural oddities, G4s are now recognized as dynamic regulatory elements of key biological processes, including transcription, replication, translation, and genome stability maintenance[1]. Notably, they are enriched in functionally relevant genomic regions, including telomeres, oncogene promoters, and untranslated regions of mRNAs[2,3]. The formation, stabilization, and resolution of G4s are controlled by a range of G4-binding proteins, such as helicases, nucleases, and transcription factors, that modulate their structure and biological activity[4]. Dysregulations of G4-protein interactions have been increasingly linked to cancer, neurodegenerative disorders, and other diseases, positioning G4s as attractive therapeutic targets[5]. In this presentation, I will show our recent efforts toward the development of small molecules and peptide-based ligands that selectively target G4 structures to interfere with their interactions with protein partners[6-9]. These studies demonstrate the potential of G4-targeting agents as tools for selective and mechanism-based drug discovery.

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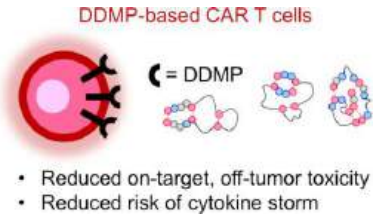
CBF - D3 - O02
Disulfide-directed multicyclic peptides for chimeric antigen receptors targeting solid tumors

Yu-Hsuan Tsai
Institute of Molecular Physiology, Shenzhen Bay Laboratory, China

The clinical application of chimeric antigen receptor (CAR) T cell therapy in solid tumors remains limited due to significant safety concerns, particularly “on-target, off-tumor” toxicity and cytokine release syndrome (CRS). Here, we describe a class of CARs that employ disulfide-directed multicyclic peptides (DDMPs) as compact antigen-recognition domains targeting the tumor-associated antigens HER2 and TROP2. DDMP-based CAR T cells exhibited antigen density-dependent cytotoxicity in vitro and in vivo, efficiently eliminating cells with high antigen expression while sparing cells with low antigen levels, thereby mitigating on-target, off-tumor toxicity. In addition, DDMP-based CAR T cells secreted markedly lower levels of pro-inflammatory cytokines upon targeted killing, reducing the CRS risk. Mechanistic analyses revealed that this favorable combination of restrained cytokine release and density-gated killing is associated with distinct T cell signaling pathway engagement and reduced cell avidity relative to conventional single-chain variable fragment (scFv)-based CAR T cells. Collectively, these findings establish DDMP-based CARs as a promising framework for engineering safer, yet efficacious, CAR T therapies for solid tumors.



We are grateful to SZBL, Shenzhen Medical Research Fund (D2501002), National Natural Science Foundation of China (22107076), and China Postdoctoral Science Foundation (2024M752146) for the financial support.

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CBF - D3 - O03

Biophysical characterization of the complex between Aβ and model peptides of optineurin: The impact of the E50K mutation in neurodegenerative pathways

Davide Deodato[1,2,6], Giulia Grasso[2], Valeria Ciaffaglione[2], Valeria Lanza[2], Giuseppina Sabatino[2], Anna Maria Santoro[2], Damiano Calcagno[1], Elisa Peroni[3], Olivier Monasson[3], Diego Sbardella[4], Grazia Raffaella Tundo[4,5], Fabio Lolicato[6], Giuseppe Grasso[1], Danilo Milardi[2]

[1]Dept. of Chemical Sciences, University of Catania, Italy; [2]CNR Istituto di Cristallografia, Sede Secondaria di Catania, Italy; [3]CY Cergy Paris Université, CNRS, BioCIS, France; [4]IRCCS Fondazione Bietti, Italy; [5]Dept. of Clinical Sciences and Translational Medicine, University of Tor Vergata, Italy; [6]Heidelberg University Biochemistry Center, Neuenheimer, Germany

Glaucoma is a chronic optic neuropathy and a main cause of irreversible blindness on a global scale. Alzheimer's Disease (AD) and Primary Open Angle Glaucoma (POAG), which is the most prevalent form of the disease, are postulated to share several pathogenic mechanisms underscoring disease onset and progression.[1,2] However, a strong connection between the two diseases remains to be firmly established.[3] This study aims at investigating the interplay between AD and glaucoma by examining the interactions between two proteins associated with their pathogenesis: Aβ and optineurin respectively. In literature, many proofs leading to the concrete possibility of their interaction can be found, but there is no experimental information regarding their affinity and its possible outcomes.[4,5] This research therefore provides unprecedented insights into the crosstalk between Aβ and optineurin, taking into consideration model peptides of both the wild-type and the E50K mutant form of the protein, which presents a missense Glu50Lys mutation and is among the most prevalent mutations harboured by subjects affected by familiar form of POAG.[6] Spectrophotometric assays along with interaction assays and molecular dynamics simulations were employed to demonstrate that such mutation and its binding to Aβ affects the oligomerization of the optineurin peptides, shedding light on the neurodegenerative mechanisms linked to glaucoma and its possible association to AD. Furthermore, it was demonstrated that both the wild-type and E50K peptides can modulate amyloid aggregation, suggesting that this interaction might be leveraged to develop new therapies aimed at reducing amyloid-related toxicity.

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CBF - D3 - O04
From planar to octahedral architectures: Geometry-driven modulation of amyloid aggregation

Sara La Manna[1], Daniela Marasco[1]
[1]*Dept. of Pharmacy, University of Naples Federico II, Italy*

Metallodrugs have attracted interest in neurological disorders for their ability to modulate amyloid protein aggregation, a hallmark of neurodegenerative diseases. They can prevent toxic oligomer formation through direct and indirect interactions with amyloid peptides.
Herein, we report on a series of metallodrugs with varying geometries, square-planar Pt(II)[1], tetrahedral Ru(II)[2], glycoconjugate pentacoordinate Pt(II)[3], octahedral Pt(IV)[4], and paddlewheel diruthenium (Ru_2^{5+})[5], and their ability to modulate the aggregation of amyloid-β ($A\beta_{1-42}$) and other amyloid model peptides.
All complexes modulated aggregation, with geometry- and ligand-dependent effects: square-planar and tetrahedral complexes influenced peptide aggregation pathways, pentacoordinate Pt(II) complexes allowed additional interactions via axial ligands, and octahedral species engaged in ligand exchange and aromatic interactions, contributing to geometry-dependent modulation.
By combining spectroscopic (fluorescence, UV–Vis and mass spectrometry), microscopic (scanning electron and confocal microscopy) techniques, and cellular assays in neuroblastoma cells, we characterized mechanisms linking complex geometry to aggregation modulation. These findings provide mechanistic insight into how metal complex geometry governs amyloid aggregation and highlight the potential of these metallodrugs as novel therapeutic scaffolds for neurodegenerative disorders.

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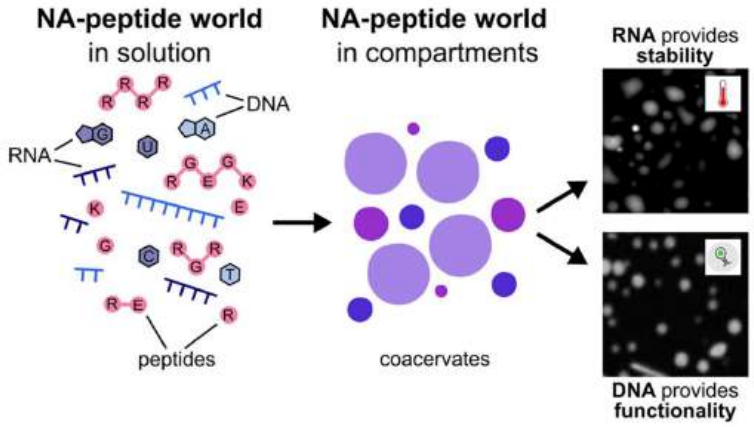
CBF - D3 - O05
Chemical requirements of coacervates as primitive cells

Fatma Z. Mihoubi[1,2*], Karina K. Nakashima[1*], Fidan Rahmatova[1,2], Claudia Bonfio[1]
[1]*Dept. of Biochemistry, University of Cambridge UK;* [2]*Institut de Science et d'Ingénierie Supramoléculaire, Université de Strasbourg, France*
**These authors contributed equally*

The early co-evolution of RNA and peptides is at the core of the RNA-peptide world hypothesis. Recent studies suggest that nucleotides and amino acids could have formed and polymerised non-enzymatically under prebiotic conditions, generating short oligonucleotides and peptides capable of non-enzymatic RNA replication and peptide synthesis. However, whether the cooperation between nucleic acids and peptides stems from their co-localisation in primitive compartments is unclear. Here we demonstrate the early and likely inevitable emergence of primitive coacervates via liquid-liquid phase separation of prebiotic heterogeneous mixtures of short non-coded oligonucleotides and peptides. We show that peptide/nucleic acid coacervates are more prone to form than peptide/peptide coacervates, and that peptide/RNA coacervates are remarkably more stable than peptide/DNA coacervates. Atomistic simulations confirm that the more extended and less structured conformation of RNA over DNA enables more contact points with peptides. The more abundant interactions in peptide/RNA coacervates lead to enhanced salt and thermal stability, yet reduced fluidity compared to their DNA counterparts - which are in turn capable to fully preserve RNA secondary structure upon partitioning. Our findings suggest that peptide/oligonucleotide co-localisation via coacervation would have inevitably occurred at an early stage of a more holistic nucleic acid-peptide world scenario. Both RNA and DNA would have thus been required to ensure the emergence of coacervates with balanced stability and fluidity to host non-enzymatic RNA chemistry.



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CBF - D3 - O06
Enhancing and probing mRNA properties via click chemistry

Sebastian Golojuch[1], Brendan Largey[1], Afaf H. El-Sagheer[1,2], Tom Brown[1]
[1]Dept. of Chemistry, University of Oxford, UK; [2]School of Chemistry, University of Southampton, UK

mRNA became a household name during the COVID-19 pandemic, but the scope of its potential therapeutic applications extends far beyond the preventive vaccines. Thanks to the mRNA modularity, it is possible to employ it, for instance, in the development of cancer immunotherapies, protein replacement therapies, and gene editing, all of which are now in clinical trials. Expanding this therapeutic repertoire, however, is not straightforward and faces challenges related to cell-type selectivity, as well as limited mRNA stability and translation efficiency. Particularly promising for optimising cell-type selectivity are mRNA designs utilising non-canonical, cap-independent translation mechanisms, for example, employing internal ribosome entry sites (IRESs). These mRNAs, however, are unstable, produce limited amounts of protein, and current methods to enhance their performance remain imperfect.

To address these challenges, we explore the use of *in vitro* transcription priming with azido-modified small-molecule reagents, which facilitate the installation of an azide handle on the 5′-end of cap-independently translated mRNAs. This azide handle enables subsequent modification of transcripts using strain-promoted azide-alkyne cycloaddition (Fig. 1). Our results[1] show that this approach can facilitate the enhancement of mRNA stability and protein output without eliciting immunogenicity. Moreover, we apply this mRNA 5′-end modification strategy to investigate transfection and cap-independent translation in cells, overcoming burdens associated with previous methods.

Together, our findings support cap-independently translated mRNAs as a viable alternative to the canonical 5′-capped transcripts and provide a modular toolkit for functional characterisation and optimisation of next-generation mRNA therapeutics.

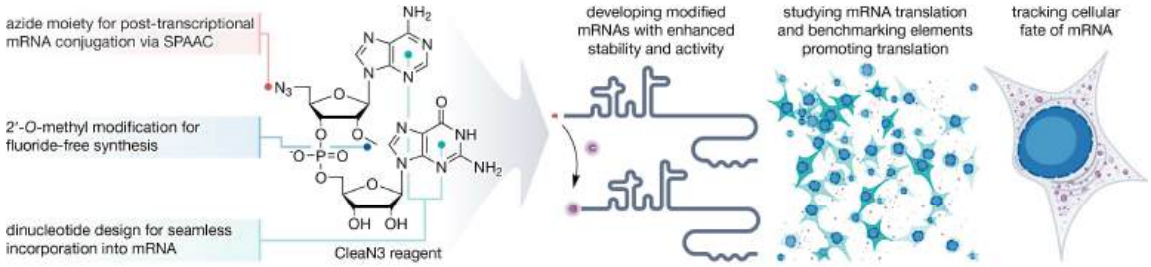

Fig. 1. An azido-modified *in vitro* transcription primer (CleaN3) enables click-mediated conjugation of cap-independently translated mRNAs to enhance and probe their properties.

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CBF - D3 - O07

Enzymatic regulation of CRISPR-Cas12a for programmable readout of DNA repair and topological states

Neda Bagheri,[1] Anna Valenti,[2] Alessandro Porchetta[1]

[1]University of Rome Tor Vergata, Italy; [2]Institute of Biosciences and BioResources, National Research Council of Italy, Italy

DNA integrity is continuously challenged by chemical damage and topological stress, both of which contribute to genome instability and cancer development. However, translating DNA repair activity and topological constraints into rapid, sensitive molecular readouts remains challenging. Here, we introduce a modular synthetic DNA transduction strategy that couples enzymatic modulation of DNA structure to programmable CRISPR-Cas12a activation. Engineered DNA constructs are designed to respond to specific enzymatic inputs-including base excision repair glycosylases and topoisomerases-by undergoing defined structural or topological transitions that that enable Cas12a target recognition. As a result, DNA damage processing and topology-regulating enzyme activities are converted into a robust fluorescence signal via Cas12a-mediated collateral cleavage, enabling molecular recognition and signal amplification in a single-step assay. The platform operates in cell lysates and can be adapted to different enzymatic inputs, providing a flexible platform for monitoring DNA repair activity and screening small-molecule inhibitors. Overall, this work establishes a general framework for enzymatic control of Cas12a activity, with potential applications in DNA repair monitoring, drug discovery, and CRISPR-based synthetic gene circuits.

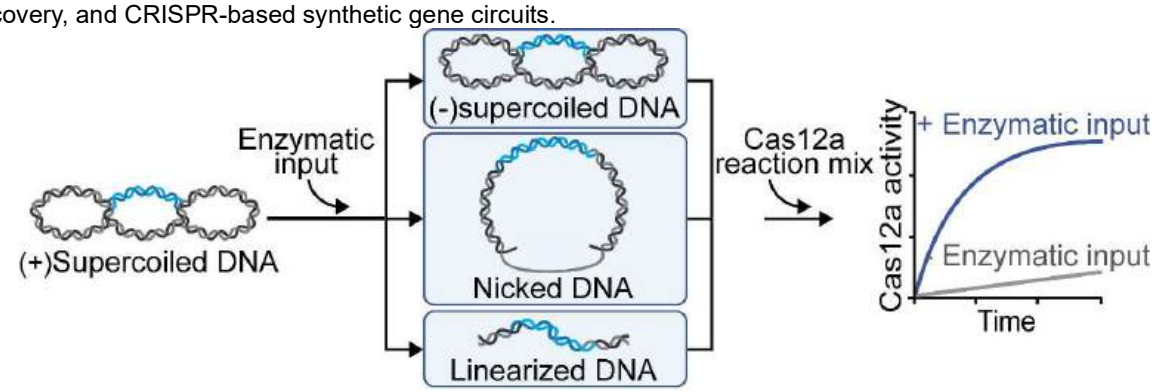

Fig. 1. Enzyme-driven modulation of DNA topology. Positively supercoiled plasmid DNA is converted to relaxed or linearized forms by enzymatic inputs resulting in restoration of Cas12a activity and signal generation.

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CBF - D3 - O08
RNA and XNA microarrays: Harnessing the full power of nucleic acid photolithography

Jory Lietard[1]
[1]*Institute of Inorganic Chemistry, University of Vienna, Vienna, Austria*

DNA microarrays are collections of nucleic acid molecules attached to a surface. Taking place directly on the array, nucleic acid synthesis *in situ* is a powerful method to access complex sequence libraries in a parallelized manner and with these libraries serving as groundwork for the assembly of genes or for the storage of digital information in DNA format. The *in situ* approach, employing classical phosphoramidite chemistry, offers high throughput in both synthesis and assays as a single experiment interrogates all sequences simultaneously.
Across academia and industry, the technology of microarray fabrication has so far only explored DNA and applications for DNA microarrays. In our lab, we have focused on demonstrating the ability to produce microarrays of any nucleic acid type, including RNA and oligonucleotide analogs [1, 2, 3]. Our array-ready chemical toolbox includes RNA, 2'-modified sugar analogs, base modifications, phosphorothioates, linkers, spacers and fluorescent dyes, and others.
The chemical and technical advances that made the expansion of the realm of microarray photolithography (Figure 1) to RNA and XNA will be exposed. The discussion will focus on the development of a new set of RNA phosphoramidites that significantly increase quality and speed in the synthesis of RNA microarrays, and how these sequence libraries can be used to study RNA aptamers. Microarrays of oligonucleotide analogs such as 2'F-ANA, L-DNA and 2'F/2'OMe RNA will also be presented along with applications in oligonucleotide drug design, surface patterning, Nanopore sequencing and enzymatic synthesis [4, 5, 6]. Using high-density microarrays, nucleic acid chemistry performed at high-throughput further illustrates the extraordinary versatility of this synthesis platform.

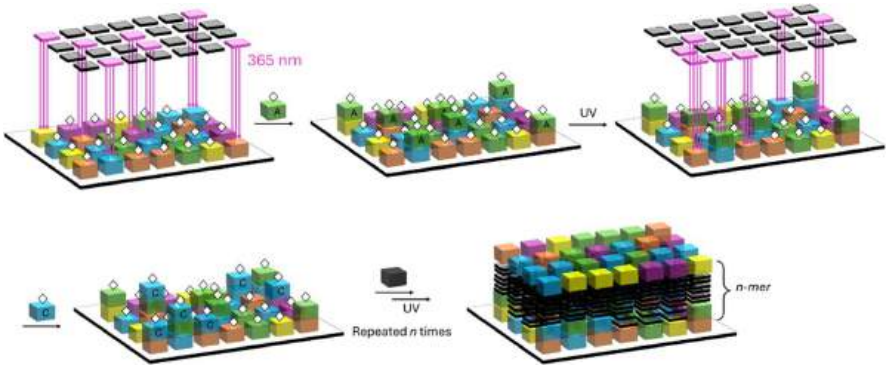

Fig. 1. Schematic description of the photolithography process where selective exposure to UV removes a terminal 5' photoprotecting group, allowing the exposed areas to couple with the next nucleotide phosphoramidite.

This ongoing research is funded by the Austrian Science Funds (FWF grants I4923, P34284 and P36203 to J.L.).

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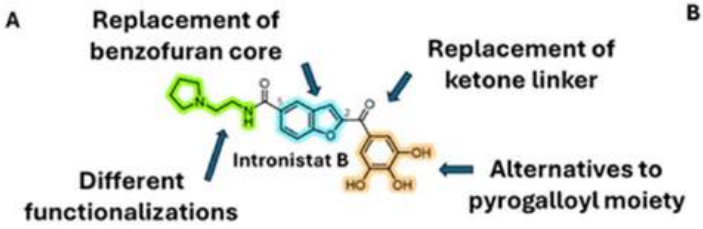
CBF - D3 - O09
Targeting (self-)splicing machineries with small molecules to fight cancer

Federico Riu[1], Nicoletta Brindani[1], Enrico Bergamaschi[1], Karina Belen Sabalette[1], Mara Di Filippo[1], Alice Triveri[1], Marco Marcia[1,2], Marco De Vivo[1]
[1]Italian Institute of Technology, Italy; [2]Dept. of Cell and Molecular Biology, Uppsala University, Sweden

For most eukaryotic genes, the pre-mRNA undergoes processing before becoming mature mRNA capable of directing protein synthesis. One key step in this process is RNA splicing, which removes intervening sequences (introns) and joins the coding sequences (exons).[1]
Among intron types, group I and II introns are self-splicing and found in bacteria, protists, and fungi. Type III (spliceosomal) introns rely on a large ribonucleoprotein complex, the spliceosome, and are present in most eukaryotic nuclear pre-mRNAs. The spliceosome plays a crucial role in pre-mRNA maturation and the regulation of gene expression. Its dysregulation is strongly linked to diseases such as cancer. Aberrant splicing contributes to multiple cancer hallmarks. Notably, small molecules targeting cancer-specific splicing factors have shown promise in overcoming drug resistance, highlighting the therapeutic potential of spliceosome modulators that enhance anticancer efficacy while minimizing adverse effects.[2]
More in-depth, inhibitors targeting the catalytic core of the splicing machinery can become selective spliceosome modulators with superior anticancer potential. This concept is supported by our recent mechanistic studies, which elucidated the catalytic function of self-splicing group II introns as evolutionary ancestors of the spliceosome. Crystallographic studies revealed that splicing can be modulated by small molecules acting at the catalytic core, demonstrating an unprecedented mode of splicing inhibition.[3-4]
Based on our recent co-crystal structures and novel compounds acting at the catalytic site, we synthesized a new class of derivatives and evaluated their splicing modulatory activity using high-throughput FRET-based assays, X-ray crystallography, and gene-reporter systems in mammalian cell lines. Drug-like properties, including chemical, metabolic, and plasma stability, have also been evaluated.[3-4]
We have identified group II intron inhibitors with sub-micromolar activity, as compound **1** with IC_{50} = 0.5 μM, and solved their structures at the site of action. Based on these results, we are working on yielding potent and selective spliceosome inhibitors with enhanced anticancer efficacy.

A



B

Compound #	IC_{50} (μM)
1	0.5 ± 0.2 μM
2	1.0 ± 0.5 μM
3	1.6 ± 0.7 μM
4	2.8 ± 0.4 μM
5	3.5 ± 0.3 μM
6	6.5 ± 4.1 μM

A. Alternatives to previously identified group II intron inhibitor intronistat B[4]; B. IC_{50}s of most potent compounds of the new series of splicing modulators.

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CBF - D3 - O10

Rationale design, synthesis and pharmacological properties of fused chromenopyrazoles as CB1 ligands

Catarina M. Correia[1,2*], Rebeca Diez-Alarcia[2,3], Carlos Cruz[4,5], Javier Vázquez[4], F. Javier Luque[5], Artur M. S. Silva[1], Luis F. Callado[2,3], Vera L. M. Silva[1]

[1]*LAQV-REQUIMTE and Dept. of Chemistry, University of Aveiro, Aveiro, Portugal;* [2]*Dept. of Pharmacology, University of the Basque Country, UPV/EHU, Leioa, Spain;* [3]*Centro de Investigación Biomédica en Red de Salud Mental, CIBERSAM, Spain;* [4]*Pharmacelera, Parc Científic de Barcelona, Spain;* [5]*Faculty of Pharmacy and Food Sciences, Instituto de Biomedicina e Instituto de Química Teórica y Computacional, Universidad de Barcelona, Spain*

The endocannabinoid system (ECS) plays a central role in the regulation of several physiological processes and has gained increasing attention as a key modulator of the neuroinflammatory pathways involved in neuropsychiatric diseases. The type 1-cannabinoid receptor (CB1R) represents a major therapeutic target for the modulation of pain, inflammation, and central nervous system disorders. Thus, modulation of the ECS by CB1 ligands stands up as a foremost therapeutic approach.[1] Therefore, developing new cannabinoids as drugs for the treatment of several diseases is a hot research topic nowadays. Pyrazoles are five-membered heteroaromatic compounds that exhibit diverse pharmacological activities, including cannabinoid activities, and serve as crucial intermediates in organic synthesis.[2] In this work, we report the design, molecular docking, synthesis, and pharmacological evaluation of a series of chromeno[3,2-*c*]pyrazol-9(1*H*)-ones and 2,4-dihydrochromeno[3,4-*c*]pyrazoles, as potential CB1 ligands. Molecular docking studies, performed to investigate the binding modes of the designed compounds within the CB1R-orthosteric binding pocket, revealed favorable interactions with key amino acid residues involved in CB1 ligand recognition, suggesting a high affinity for the receptor. The target compounds were synthesized through efficient synthetic protocols, involving the reaction of hydrazones **1** with 3-nitrochromenes **2**, or 3-bromochromones **4** to afford structurally diverse-fused chromenopyrazoles **3** and **5**, respectively, in good yields (**Fig.1**), whose chemical structures were confirmed using standard spectroscopic techniques. Pharmacological evaluation using *in vitro* radioligand competition binding and [^{35}S]GTPgS assays showed that several derivatives exhibited significant CB1R binding affinity and functional activity, with distinct profiles depending on the substitution pattern. Overall, this study identifies fused chromenopyrazoles as promising templates for the development of new CB1 ligands and provides valuable insights into their structure–activity relationships, supporting further optimization towards therapeutically relevant CB1R modulators.

Fig.1. Molecular docking studies and synthesis of 2,4-dihydrochromeno[3,4-*c*]pyrazoles (**3**) and chromeno[3,2-*c*]pyrazol-9(1*H*)-ones (**5**).

Funding and Acknowledgments: This work was funded by FEDER–Fundo Europeu de Desenvolvimento Regional funds through the COMPETE 2030 and by Portuguese funds through FCT–Fundação para a Ciência e a Tecnologia in the framework of the project COMPETE2030-FEDER-00792200. Thanks are also due to the University of Aveiro and PT national funds (FCT/MCTES, Fundação para a Ciência e Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) through the project UID/50006/2025-Laboratório Associado para a Química Verde-Tecnologias e Processos Limpos, the Basque Government (IT1512/22 and IT1920/26) and the Spanish Ministerio de Ciencia, Innovación y Universidades (PID2023-147942OB-I00 MCIN/AEI/10.13039/501100011033). Catarina M. Correia thanks FCT/MCTES for her PhD grant 2022.11584.BD. Thanks are also due to the National NMR Network (PT NMR) partially supported by Infrastructure Project No. 022161 (co-financed by FEDER through COMPETE 2020, POCI and PORL and FCT through PIDDAC).

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CBF - D3 - O11

CNS sparing agents targeting cannabinoid-1 receptors for treatment of metabolic syndrome disorders

Malliga R. Iyer*, Pinaki Bhattacharjee[2], Henry Puhl[3], Paul Volesky[2] et al

[1]Section on Medicinal Chemistry, National Institute on Alcohol Abuse and Alcoholism (NIAAA), National Institutes of Health (NIH), USA; [2]Laboratory of Biophotonics and Quantum Biology, National Institute on Alcohol Abuse and Alcoholism, National Institutes of Health, USA

Multiple GPCR signaling pathways are involved in chronic diseases like metabolic syndrome (MetS). The endocannabinoid (EC) system plays a key regulatory role in MetS pathophysiology. Metabolic syndrome stems from obesity and contributes to several comorbidities, including insulin resistance, deleterious cardiovascular events, and fibroproliferative disorders. This highlights an urgent need for novel therapeutics aimed at MetS and its related conditions. Acting primarily through its G-protein–coupled receptors, CB1 and CB2, the EC system has emerged as a validated therapeutic target for MetS-associated disorders. Notably, selective antagonism of cannabinoid receptors, especially CB1, has demonstrated effectiveness in reducing food intake, enhancing insulin sensitivity, and mitigating fibrosis. However, withdrawal of the first brain-penetrant CB1 blocker, rimonabant, from the European market due to psychiatric side effects resulted in shifting gears towards alternate approaches and treatment modalities to harness the therapeutic benefits of CB1 antagonism. Research in this realm shifted towards developing non-brain-penetrant mechanisms of CB1 blockade resulting in the revival of the CB1R MoA whose potential rivals GLP-1R-based therapies. Continued development from our lab has resulted in novel platform synthesis methods, sensor tools and lead candidates. Case study from 'chemistry to clinical candidate' involving the pyrazoline and pyridazine series of CB1 compounds will be presented.(1,2)

Acknowledgements: This work was supported by intramural funds from the National Institute on Alcohol Abuse and Alcoholism (NIAAA) to M.R.I (ZIA AA000360). This research was supported by the Intramural Research Program of the National Institutes of Health (NIH).

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CBF - D3 - O12

Molecular design of ultrabright NIR-II fluorescent probes for deep-tissue imaging

Yang-Hsiang Chan[1]
[1]*Dept. of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*

Fluorescence has been developed for over a century, and in the field of chemistry, it has long been used as an analytical tool to determine the concentrations of various neutral or ionic substances. Initially, fluorescence tracing technology found widespread application in the hydrogeological field, especially in simulating and tracing pollutant emissions. Over the past few decades, fluorescence technology has been extensively utilized for biomarking and cell labeling, shedding light on the fundamental interactions between biomolecules and studying physiological mechanisms within organisms. In recent decades, Near-Infrared II (NIR-II, 1000-1700 nm) fluorescence has gained attention in the biomedical field, as NIR-II emission implies greater tissue penetration, enabling real-time imaging of deeper tissue layers. In particular, the flourishing development of NIR-II over the past decade has had a significant impact on clinical surgery. However, the synthesis of bright NIR-II dyes remains a big challenge owing to the intrinsic energy gap law leading to low fluorescence quantum yields. This talk will explore fundamental molecular design strategies to circumvent the constraints of the energy gap law, focusing on the synthesis of novel, bright NIR-II emissive fluorophores. Furthermore, we will discuss state-of-the-art NIR-II deep-tissue imaging techniques and their potential to redefine the future of bio-imaging and precision medicine.

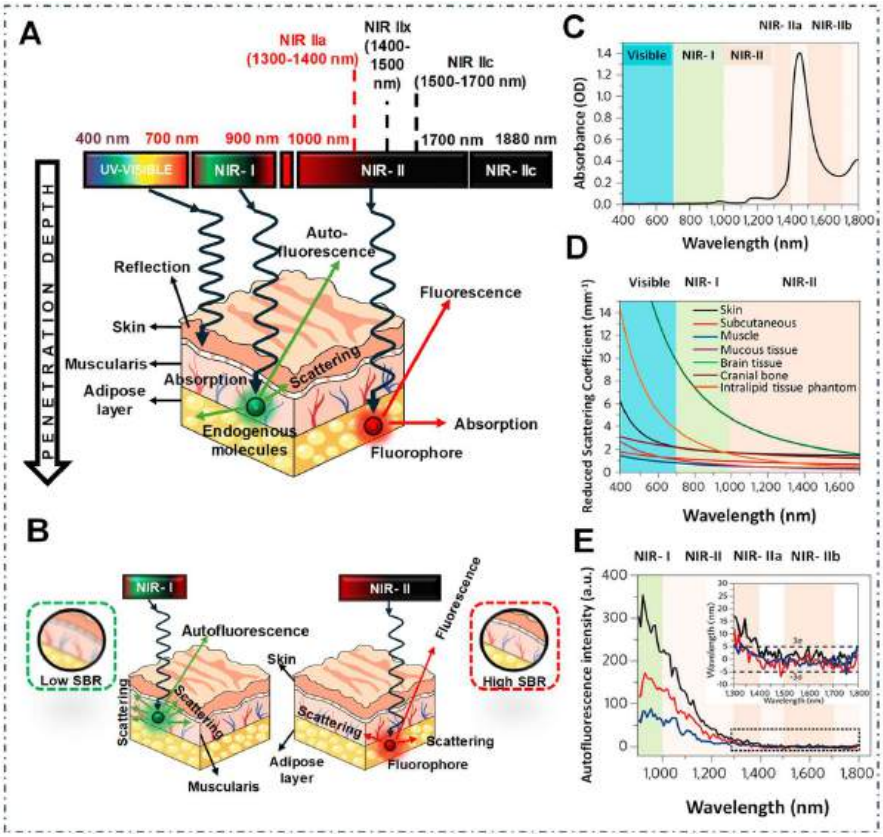

Fig. 1. Advantages of NIR-II Imaging for in vivo.

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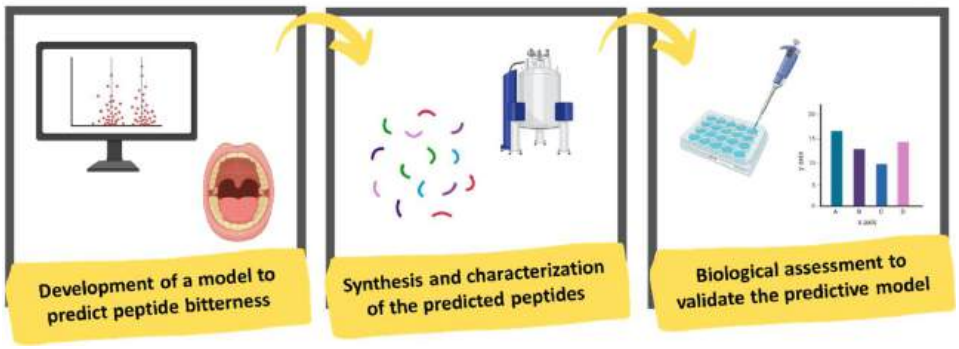
CBF - D3 - O13

From prediction to bench: An integrated modelling–synthesis framework for bitter peptide identification

Kelly Bugatti[1], Francesco Ferri[2], Tullia Tedeschi[1], Antonella Di Pizio[2]
[1]University of Parma, Dept. of Food and Drug. Italy; [2]Leibniz Institute for Food Systems Biology at the Technical University of Munich. Germany

Taste is a critical determinant of food acceptance and plays a central role in shaping dietary habits. During food processing, proteins can release peptides, including chemically modified structures, that frequently elicit undesirable bitter sensations. Early prediction of peptide bitterness is therefore essential to guide process optimization and support the development of alternative proteins.[1,2]

Representing chemically diverse peptides remains a major challenge for predictive modelling. Traditional formats such as FASTA capture only primary sequence information and overlook structural complexity, including non-canonical residues, backbone modifications, and cyclization. To address this limitation, we employed the Boehringer Ingelheim Line Notation (BILN), a chemically expressive format that enables the development of machine-learning models grounded in realistic molecular structure while keeping computational overhead minimal.



To experimentally validate and refine the computational predictions, a representative panel of peptides, both predicted bitter and non-bitter, was synthesized via solid-phase peptide synthesis. All compounds were purified by preparative HPLC and fully characterized by mass spectrometry and NMR spectroscopy to confirm identity, purity, and structural integrity. The synthesized peptides were subsequently evaluated *in vitro* for their binding affinity across the full panel of human bitter taste receptors (TAS2Rs), generating a receptor-level map of predicted versus observed activity. In parallel, selected sequences underwent controlled sensory evaluation to assess their perceived bitterness under realistic tasting conditions.

The continuous exchange between computational modelling and synthetic validation was fundamental: experimental data informed iterative refinement of the predictive model, while computational output guided the selection of structurally diverse candidates for synthesis.

By integrating expressive chemical notation, machine learning, synthetic and sensory validation, this work establishes a robust framework for understanding and predicting peptide bitterness, ultimately supporting improved sensory quality and consumer acceptance in emerging food systems.

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CBF - D3 - O15

Integrating chemical and biological knowledge to enhance translational research: Insights from recent studies

Marta Da Pian[1], Giulia Moncelsi[2]
[1]Elsevier GmbH, Germany; [2]Elsevier Srl, Italy

Recent studies, including investigations on substrate- and product-selective supramolecular catalysis[1] and systematic analyses of epigenetic mechanisms underlying stress-induced vulnerability to depression[2], illustrate the increasing need for integrating chemical and biological data to advance mechanistic understanding and translational research.

We present an approach that connects experimental findings with curated chemical, biological, and pharmacological knowledge from databases such as Reaxys, Embase, Pharmapendium, and Embiology. By systematically integrating published data with these resources, it is possible to enhance reproducibility, generate mechanistic hypotheses, and identify patterns that span chemical and biological systems.

This framework demonstrates how combining experimental insights with structured knowledge supports decision-making in chemical biology and drug discovery. It highlights the potential of integrated data to accelerate mechanistic understanding, inform translational strategies, and provide a coherent view of complex chemical–biological interactions beyond individual studies.

Acknowledgements: This work would not have been possible without the scientific rigor, insight, and contributions of our co-authors, whose expertise was essential in shaping the experiments, analyses, and interpretations presented here.

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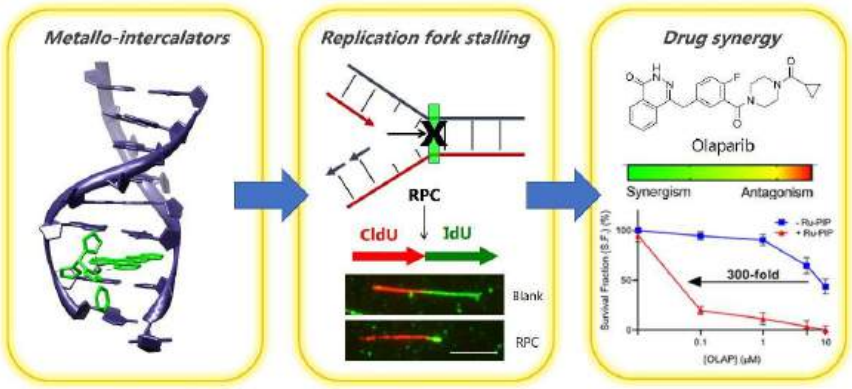
CBF - D3 - O16
Combining ruthenium(II) metallo-intercalators and PARP inhibitors for cancer therapy

Martin R. Gill[1], Nur Ainine Yusoh[2], Xiaohe Tian[2], Haslina Ahmad,[3]
[1]Swansea University, UK; [2]Sichuan University, China; [3]Universiti Putra Malaysia, Malaysia

Poly(ADP-ribose) polymerase inhibitors (PARPi) have achieved notable clinical success in treating cancers by exploiting deficiencies in DNA repair pathways; however, their efficacy is largely confined to a relatively small percentage of tumours that harbour BRCA mutations, thereby restricting their clinical use. Due to this, small molecules able to function as "PARPi sensitizers" hold substantial promise within PARPi combination therapy.[1] Ruthenium(II) polypyridyl complexes (RPCs) have emerged as a versatile class of metallo-intercalators that reversibly bind duplex DNA and inhibit cell proliferation through mechanisms distinct from cisplatin accompanied by reduced genotoxicity.[2] Here we describe a novel therapeutic approach that combines RPCs with PARPi to overcome resistance in BRCA-proficient cancers and expand the use of PARPi to include BRCA-proficient subtypes. Motivated by $[Ru(dppz)_2(PIP)]^{2+}$,[3,4] we have utilised a mix of molecular design of close structural derivatives and small library screening to show that the distinct DNA damage response generated by RPC metallo-intercalator replication fork stalling acts to sensitize cancer cells to PARP inhibition, producing enhanced double-strand break accumulation and apoptotic signalling in target cancer cells, overall resulting in a synthetic lethal interaction independent of BRCA status.[5,6]
The findings highlight the potential of ruthenium-based chemotypes to expand the scope of PARP inhibitor therapy beyond current genetic restrictions, providing a platform for rational combination regimens in precision oncology.



We thank Cancer Research Wales and the Welsh Government for funding.

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CBF - D3 - O17

Combining boron and gadolinium neutron capture therapy with the inhibition of carbonic anhydrase for the treatment of mesothelioma

Polyssena Renzi[1], Alberto Lanfranco[1], Sahar Rakhshan[2], Diego Alberti[2], Aida Zarechian[2], Sabrina El Khanoufi[2], Nicoletta Protti[3,4], Simonetta Geninatti Crich[2], Anammaria Deagostino[2]

[1]Dept. of Chemistry, University of Torino, Italy; [2]Dept. of Molecular Biotechnology and Health Sciences, University of Torino, Italy; [3]Dept. of Physics, University of Pavia, Italy; [4]Nuclear Physics National Institute (INFN), Unit of Pavia, Italy

Malignant pleural mesothelioma (MPM) is a disseminated tumor for which conventional radiotherapy lacks effectiveness. Despite the ban on asbestos introduced by law, the number of deaths and new cases is still high due to the long latency period. New treatments are available but the median overall survival is still one year.[1] A possible therapeutic option relies on Neutron Capture Therapy (NCT),[2] a binary radiotherapy based on the capture reaction of thermal neutrons by various nuclides, e.g. ^{10}B and ^{157}Gd, mainly employed in the treatment of malignant tumors. ^{10}B is a non-radioactive and non-toxic isotope, which, upon NC, undergoes fission generating ^{7}Li and α-particles, releasing their energy in path lengths comparable to a mammalian cell. ^{157}Gd is the stable nuclide with the highest NC-cross section. Neutron absorption results in the emission of γ-rays and Auger electrons. Moreover, Gd is paramagnetic and can be used as MRI contrast agent, allowing for precise neutron irradiation. Here, we report our finding on combining BNCT with carbonic anhydrase (CA) inhibition to treat MPM.[3] CA enzymes regulate pH in tumours and are involved in chemoresistance. Pivoting on our studies of functionalised carboranes as theranostic agents, we developed novel multivalent agents for the treatment of MPM integrating BNCT, GdNCT, and CA inhibition (**Figure 1**).

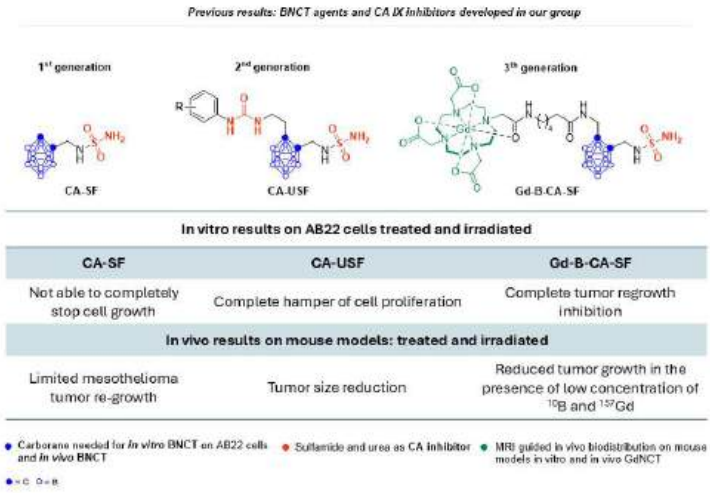

Fig. 1. Evolution of the agents used as NCT-CA inhibitors and their *in vivo* and *in vitro* results in mesothelioma treatment.

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CBF - D3 - O18

Combination of antimalarial drugs with natural acidic lipids delivers surface-active ionic liquids with multi-stage antimalarial activity

Ricardo Ferraz[1,2,3*], Ana Teresa Silva[1#], Isabel S. Oliveira[4], Inês Morais[5], Sofia Santana[6], Eyob A. Workneh[6], Miguel Prudêncio[6], Fátima Nogueira[5], Eduardo F. Marques[4], Paula Gomes[1]

[1]LAQV-REQUIMTE, Depto de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Portugal; [2]Ciências Químicas e das Biomoléculas, Escola Superior de Saúde - Instituto Politécnico do Porto, Portugal; [3]Centro de Investigação em Saúde Translacional e Biotecnologia Médica (TBIO)/Rede de Investigação em Saúde (RISE-Health), Escola Superior de Saúde, Instituto Politécnico do Porto, Portugal; [4]CIQUP, IMS (Institute of Molecular Sciences), Depto de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Portugal; [5]Universidade NOVA de Lisboa, UNL, Global Health and Tropical Medicine, GHTM, Associate Laboratory in Translation and Innovation Towards Global Health, LAREAL, Instituto de Higiene e Medicina Tropical, IHMT, Portugal; [6]Instituto de Medicina Molecular, Faculdade de Medicina Universidade de Lisboa, Portugal

Malaria eradication is included in Target 3.3 of Goal 3 under the UN Sustainable Development Agenda for 2030. Despite some progress, most antimalarials act on a single stage and face rising resistance. We have recently explored a strategy to improve antimalarial drugs using simple and affordable approaches. One approach was based on combining basic antimalarial drugs with natural acidic lipids to produce ionic liquids (IL) that might show enhanced physicochemical and biological properties compared to the parent drugs. As such, chloroquine and primaquine were paired with fatty acids and with bile acids, chosen for their biocompatibility and amphiphilic nature, which could lead to self-assembling, surface-active ionic liquids (SAIL).

The salts resulting from pairing primaquine with fatty acids were comparable or superior to the parent drug regarding the liver and blood-stage antiplasmodial activity, respectively. The salts produced by combination of chloroquine with the fatty acids showed improved blood-stage activity, with the laurate derivative showing an 11- and 6-fold increase in potency against, respectively, chloroquine-sensitive and chloroquine-resistant *P. falciparum* strains. Relevant results were obtained when pairing with bile acids. Thus, primaquine-derived salts preserved the liver-stage activity, while those derived from chloroquine retained blood-stage activity and, remarkably, showed increased liver-stage activity and gametocytocidal action. Surface tension studies were conducted to assess the surface-activity of the salts produced, demonstrating their ability to behave as SAIL. Chloroquine-bile SAILs were further combined with F127 block copolymer micelles, resulting in a nanocarrier with improved blood-stage antiplasmodial activity.

Overall, these findings support the potential of drug-derived ILs as an effective strategy for revitalizing established ionizable drugs.

Funding: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

CBF - D3 - O19

Development of a dual-functional nanostructure for simultaneous plasmonic heating and real-time temperature sensing

Jordi Jaenen[1], Anna M. Kaczmarek[1]
[1]NanoSensing Group, Ghent University, Belgium

Gold nanorods (AuNRs) have gained a lot of interest towards photothermal therapy (PTT) for cancer treatment due to their tunable localized surface plasmon resonance (LSPR) falling within the biological windows (BWI: 700–950 nm and BWII: 1000–1350 nm). Upon excitation, AuNRs generate heat that is dissipated to their surroundings resulting in cancer cell death.[1] Precise monitoring of local cellular temperature during PTT is crucial to avoid damage to surrounding healthy cells.

Determining temperature changes at the nanoscale has been the focus of the field of luminescent based nanothermometers. Up to date, a diverse range of lanthanide-doped luminescent nanothermometers with well-defined excitation and emission regions has been developed. These nanothermometers provide high thermal sensitivity, spatial and spectral resolutions.[2] The application of NIR nanothermometers is beneficial as it improves light penetration through tissue by providing luminescence in the BWs.

In this work, a hybrid composite consisting of a silica core serving as a platform decorated with AuNRs for light-to-heat conversion and Ho^{3+},Yb^{3+} doped nanoparticles for local temperature monitoring is presented.[3] Combining both heating and temperature sensing functionalities in one single hybrid composite offers a promising solution for real-time thermal feedback during treatment.[4] This approach demonstrates great potential for advanced therapeutic strategies requiring localized thermal control.

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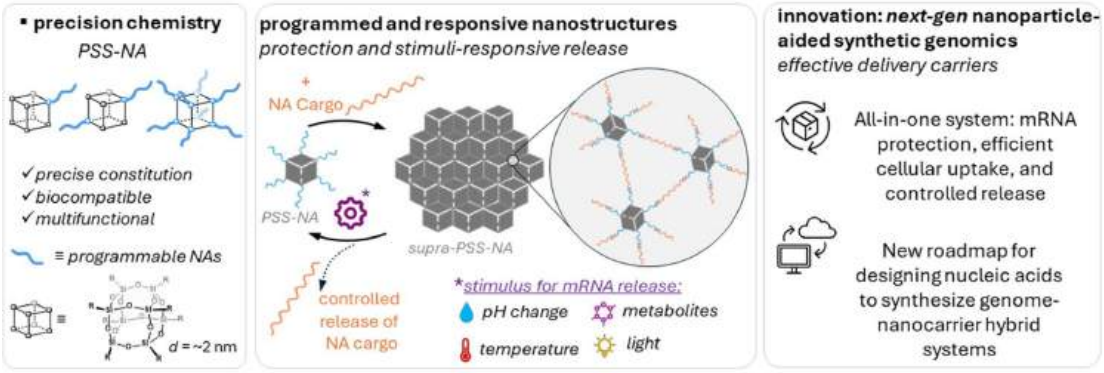
CBF - D3 - O20
Silsesquioxane-nucleic acids suprastructures for controlled gene therapy

Rabia Zahid[1], Laura Beltrán Chamorro[2], Alessandro Porchetta[3], Pierre Picchetti[4]
[1]Karlsruhe Institute of Technology (KIT), Germany; [2]University of Rome Tor Vergata, Italy; [3]University of Rome Tor Vergata, Italy; [4]Karlsruhe Institute of Technology (KIT), Germany

Multi-stimuli-responsive nanoparticles that emulate key features of biological self-assembly are a crucial step toward a new generation of adaptive nanomaterials.[1] In particular, such systems could help unlock advanced therapeutic concepts, including precision gene therapy.[2] However, current nanocarriers often lack dynamic, stimuli-dependent control over the release and stabilization of biomolecular cargos such as nucleic acids.[3] To address this limitation, we present a modular nano-delivery platform in which polyhedral silsesquioxanes (PSS) are functionalized with nucleic acids (NAs) to form well-defined supramolecular assemblies via reversible, stimulus-triggered interparticle aggregation. PSS are ultrasmall (≤ 2 nm), chemically precise inorganic cages with symmetrically arranged reactive vertices that allow programmable assembly with complementary strands, including mRNA, into supraparticles (supra-PSS-NA) capable of efficiently shielding sensitive gene-therapy cargos from mechanical and enzymatic degradation. Beyond nucleic acids, these nanostructures can be decorated with additional functional units, such as contrast agents or catalytic motifs, opening new possibilities for multimodal, theranostic applications.



The authors acknowledge the financial support from the Fonds der Chemischen Industrie des Verbandes der Chemischen Industrie e. V. (VCI) for the Liebig-Stipendium, which has enabled significant contributions to this research.

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CBF - D3 - F02

A multi-omics approach to understand how cold atmospheric plasma affects patient-derived head and neck and pancreatic tumors

Jana Baroen[1,2], Emma Peeters[1], Axelle Van der Voort[1], Lisa Van der heyden[1], Hanne Verswyvel[1], Hannah Zaryouh[1], Sofie Seghers[1], Maxim Le Compte[1], Felicia Rodrigues Fortes[1], Geert Roeyen[1,3], Vera Hartman[3], Gilles Van Haesendonck[1,3], Hans Prenen[1,3], Senada Koljenovic[1,3], An Wouters[1], Christophe Deben[1], Steven Van Laere[1], Jonas Van Audenaerde[1], Angela Privat-Maldonado[1], Inge Mertens*[1,2], Evelien Smits*[1], Annemie Bogaerts*[1]

[1]University of Antwerp, Antwerp, Belgium; [2]Environmental Intelligence Unit, Flemish Institute for Technological Research (VITO), Mol, Belgium; [3]Antwerp University Hospital, Antwerp, Belgium

** Shared senior author*

Head and neck squamous cell carcinoma (HNSCC) and pancreatic ductal adenocarcinoma (PDAC) are among the most aggressive cancers. Pancreatic cancer is projected to become the second leading cause of cancer-related deaths by 2030, while head and neck cancer is in the top 10. Despite available treatments, 5-year survival remains poor, around 10% for PDAC and 60% for HNSCC, highlighting the need for new therapeutic strategies.[1,2]

In this study, we investigate **cold atmospheric plasma (CAP)**, an emerging technology that uses ionized gas at room temperature to selectively damage cancer cells. To evaluate its effects, we use **patient-derived tumor organoids (PDTOs)**, miniature, three-dimensional models grown from patients' tumors. Unlike flat cell cultures, these organoids preserve the structure and genetic diversity of tumors, making them a powerful tool for studying treatment responses.[3]

We apply a **multi-omics approach**, combining DNA sequencing, RNA sequencing, and proteomics to examine CAP-induced changes at the genomic, transcriptomic, and protein levels. This comprehensive analysis allows us to uncover molecular mechanisms that drive sensitivity or resistance to CAP and to understand how differences between patients influence treatment outcomes.

By providing a systems-level view of CAP effects in clinically relevant models, this work aims to inform the development of **personalized plasma-based therapies**. Ultimately, these insights could help identify which patients are most likely to benefit from CAP and guide its integration into precision oncology.

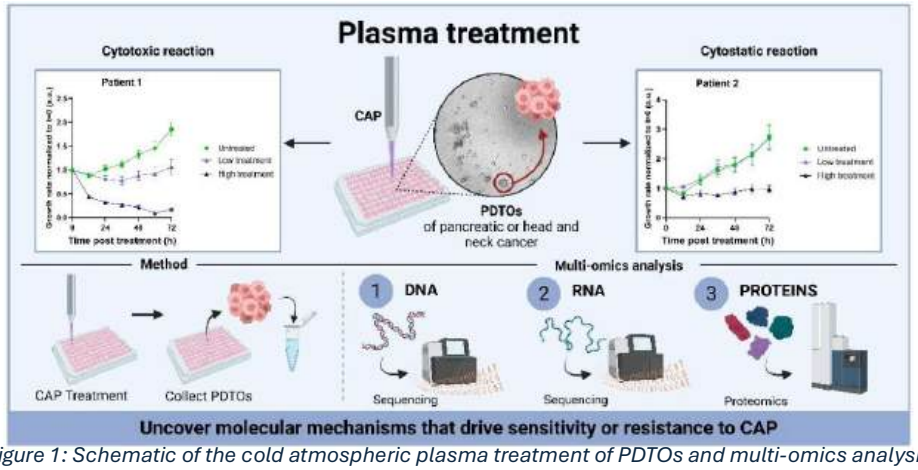

Figure 1: Schematic of the cold atmospheric plasma treatment of PDTOs and multi-omics analysis

This work was supported by the UAntwerp-Methusalem project of A. Bogaerts, a research grant from VITO and several donations. E.P. holds a fellowship of Research Foundation Flanders.

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CBF - D3 - F03

Characterisation of *Brucella melitensis* phosphoserine phosphatase through crystallographic and kinetic studies

Tanguy Scaillet[1], Johan Wouters[1]
[1]Laboratoire de Chimie Biologique Structurale (CBS), Namur Institute of Structural Matter (NISM), Namur Research Institute for Life Sciences (NARILIS), University of Namur (UNamur), Belgium

Brucella melitensis is a pathogenic intracellular bacterium causing brucellosis, a chronic infectious disease affecting sheep and goat flock. It can also affect humans after consumption of contaminated products or contact with infected animals[1,2]. Previous studies carried out by Révora *et al* with an ortholog of *Brucella melitensis* (*Brucella abortus*, 99% sequence identity) demonstrated that these bacteria cannot replicate without L-serine and that the phosphoserine phosphatase enzyme is essential for bacterial replication[3]. Targeting this enzyme could therefore represent a strategy to limit the bacteria propagation.
The main goal of the presented work is to achieve a better understanding of the phosphoserine phosphatase from *Brucella melitensis* to evaluate its potential as a therapeutic target. To this end, the enzyme was studied using kinetic and crystallographic approaches. The first three-dimensional structure of the enzyme was obtained (Figure 1). A detailed analysis of the phosphoserine phosphatase was performed by studying the enzyme in complex with its natural substrates and products, as well as with substrate and cofactor analogues, allowing a deeper insight into the molecular determinants governing catalysis and ligand recognition.

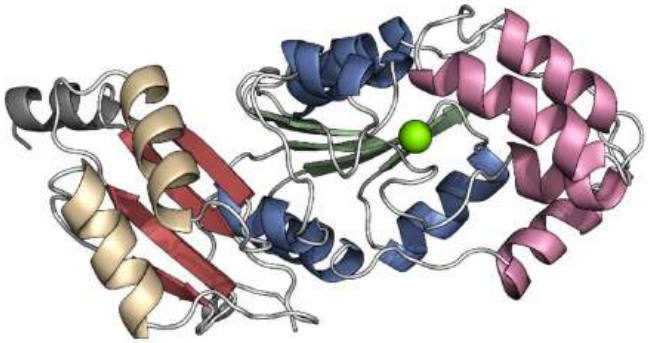

Fig.1. First 3D structure of Brucella melitensis phopshoserine phosphatase (PDB: 9FQ5)

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CBF - D3 - F04

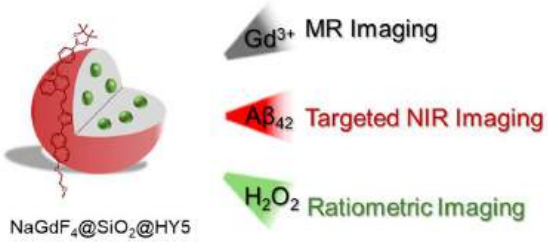
Multimodal nanoprobe for amyloid-β targeted imaging and oxidative stress monitoring in Alzheimer's disease

Yuncong Yang[1], Chengke Wang[2], Man Shing Wong[1]

[1]Dept. of Chemistry, Hong Kong Baptist University, Kowloon Tong, Hong Kong, SAR China; [2]School of Food Engineering, Ludong University, Yantai, China

Alzheimer's disease (AD) is characterized by progressive impairment of cognitive functions and memory loss due to irreversible degeneration of synapses and neuronal loss. Oxidative stress caused by the overproduction of reactive oxygen species (ROS) has been shown to be closely associated with the presence of amyloid-β (Aβ) aggregates, the pathological hallmark of AD. However, tools that can simultaneously detect and monitor the levels of oxidative stress and Aβ aggregates are rare, which are vital for early disease diagnosis, etiological investigations, and treatment assessment of the developed drugs. Toward this end, we present herein a novel approach to develop a smart multimodal nanoprobe being able to conduct Aβ-targeted NIR imaging, ratiometric sensing of H_2O_2, and magnetic resonance (MR) imaging of Aβ aggregates in a single entity for precise disease diagnosis and prognosis of AD. To integrate all these imaging functions together, a highly sensitive, Aβ-specific H_2O_2-responsive ratiometric NIR fluorescent probe that can apply for real time visualization of H_2O_2 level induced by Aβ ratiometrically in AD cell and mouse models was first developed. Meanwhile, paramagnetic $NaGdF_4$ nanoparticles (NPs) were synthesized to acquire magnetic properties for MRI. The freshly prepared $NaGdF_4$ NPs were then protected by a mesoporous silica layer in which the developed H_2O_2-responsive probes were deposited onto the surface of the NPs leading to a H_2O_2-responsive NIR/MR multimodal imaging nanoprobe. This multimodal nanoprobe was shown to be able to target Aβ and visualize ratiometrically the endogenous H_2O_2 level in an AD cell model. Furthermore, this responsive nanoprobe was highly sensitive to ratiometrically detect and monitor the Aβ-induced H_2O_2 level in APP/PS1 AD mouse model in real time with several age groups over time. Most importantly, this Aβ-targeted nanoprobe was shown to be an effective MRI contrast agent for *in vivo* T_1-weighted MRI of Aβ content in an AD mouse model.

Figure 1. A multimodal nanoprobe capable of conducting Aβ-targeted NIR imaging, ratiometric sensing of H_2O_2, and magnetic resonance imaging of Aβ aggregates.



CBF - D3 - F05
Polyphenolates as bipotent photostabilising and solubilizing agents for riboflavin

Eva Mueller[1], Nadja Ulmann[1] Didier Touraud[1], Werner Kunz[1]
[1]*University of Regensburg, Institute of Physical Chemistry, Germany*

We recently demonstrated that natural antioxidants, owing to their specific intermolecular interactions, can act as highly efficient hydrotropes for otherwise polar yet π-stacking compounds. As a model system, we investigated the photostability of riboflavin (vitamin B_2) in water in the presence of different polyphenolates over a broad concentration range.[1]
Our most recent results highlight that natural polyphenolates can likewise function as efficient photostabilizers through concentration-dependent, non-classical mechanisms that are distinct from simple radical scavenging. This dual role as solubilizers and photoprotective agents opens new perspectives for the formulation of light-sensitive ingredients in food, nutraceutical, and cosmetic systems.
We found the photostability of riboflavin to strongly depend on both the chemical nature and the concentration of the polyphenolates. In the diluted regime (molar ratios 6–50), the presence of polyphenolates slowed riboflavin photodegradation by a factor of 2–4 compared to pure aqueous solutions. At high polyphenolate concentrations, complete photostabilization of riboflavin was achieved, even after prolonged light exposure of 8 and up to ≥12 weeks.
Analysis of the photodegradation products implied that different mechanisms govern photoprotection at low and high hydrotrope concentrations. Importantly, the antioxidant capacity of selected polyphenolates could be excluded as the dominant factor responsible for riboflavin stabilization.

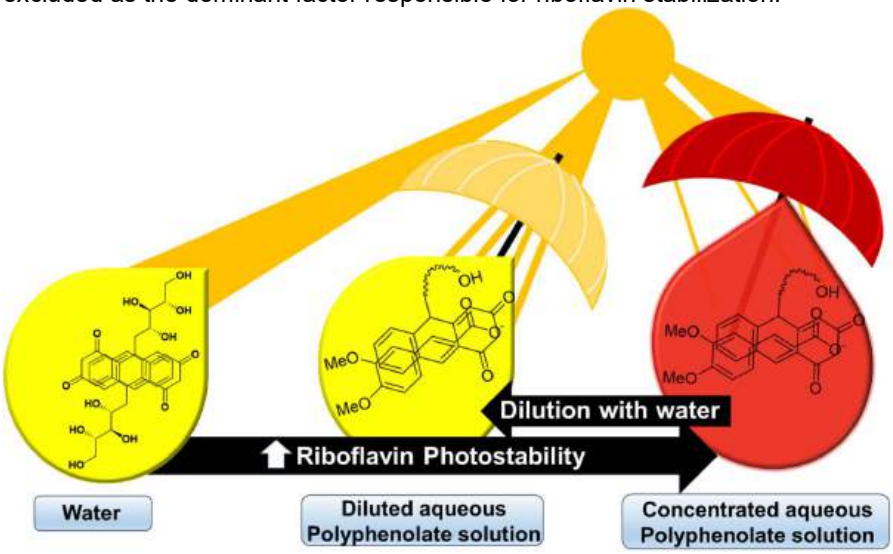


Fig. 1. Schematic drawing of the increased photostabilization of riboflavin in water at different concentrations with the help of natural antioxidative hydrotropes as solubilizers.

We thank BASF for financial support.

[1]Ulmann, N.; Hioe, J.; Touraud, D.; Müller, E.; Horinek, D.; Kunz, W. *Journal of molecular liquids* **2025**, *426*, 127465. DOI: 10.1016/j.molliq.2025.127465.

CBF - D3 - F06
Development of oligonucleotide probes to study the enzyme SNM1A

Fayanne Nolin[1], Mark Berney[1,2,3], Mary Flood[2], Ellen Fay[1], William Doherty[1], Steven Ferguson[2], Joanna McGouran[1]
[1]Trinity College Dublin, Ireland; [2]University College Dublin, Ireland; [3]Queen's University Belfast, UK

SNM1A is a DNA damage repair enzyme that repairs cytotoxic interstrand crosslinks (ICLs).[1] However, SNM1A overexpression is associated with resistance to ICL-inducing chemotherapeutics like cisplatin.[1] This work aims to develop probes targeting the metalloenzyme SNM1A by using motifs that mimic and bind strongly the active site. A terminal 5'-phosphate is vital for nuclease activity, and a $Zinc^{2+}$ ion is in the active site[2] (Fig. **1**).

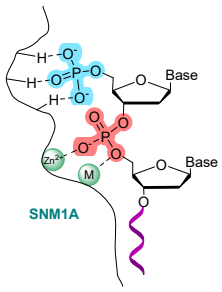


Fig. 1. Structure and Binding of SNM1A with Natural DNA

The first probe design uses thymidine dimers in which Zinc-binding groups (ZBGs) replace the native phosphodiester (PO) linkage between two nucleosides (red, Fig. **2a**). Substitution of the natural backbone with ZBGs allows chelation of the $Zinc^{2+}$ ion in the active site, thus preventing strand cleavage. Modified thymidine dimers presenting urea, sulfanylacetamide, sulfinylacetamide, squaramide, oxyurea and oxyamide ZBGs have been incorporated into an oligonucleotide strand *via* either PO or phosphorothioate (PS) linkages (green R^2, Fig. **2a**) using solid-phase synthesis.
Preliminary assays of 16 modified oligonucleotides identified 3 strong SNM1A binders: 5'-phosphorylated sulfanylacetamide with PO linkage, 5'-alcohol urea with PS linkage, and 5'-phosphorylated oxyurea with PO linkage (Fig. **2b**).

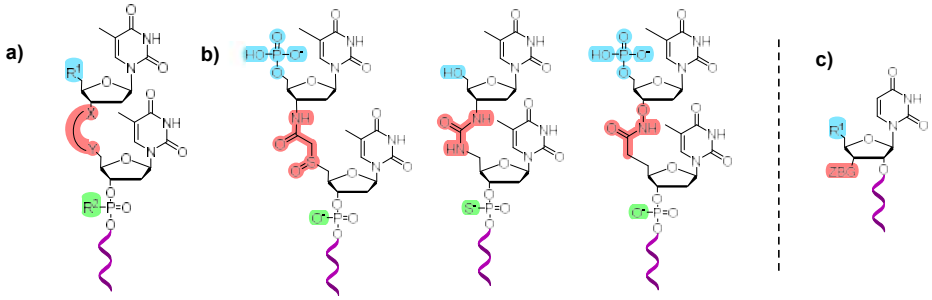


Fig. 2. **a)** Design of internucleotide ZBG Probe. **b)** 3 Oligonucleotide Probes Exhibiting Strong Binding to SNM1A. **c)** Probe Incorporating a 3'-ZBG and a 2'-5' Linkage to 20mer

A second probe design involves modified uridine monomers bearing a ZBG at the 3' position, and a 2'-DNA strand, replacing the canonical 3'-5' phosphodiester bond (**Fig. 2c**). The additional 2'-alcohol allows further functionalization to investigate optimal positions for SNM1A binding.
Three 3'-ZBGs (squaramide, sulfonamide, thiophene) were synthesized from a 3'-amine in 6 steps. An additional 4 steps allowed DNA incorporation by obtaining their phosphoramidite versions. Current targets in development include a 3'-hydrazine and 3'-hydroxamic acid moieties.
Developing the first SNM1A probes will enable research into this protein biochemistry and assist drug discovery through 3D structure elucidation of probe bound SNM1A and inhibitor screening.

[1]Bielinski, M.; Henderson, L. R. *et al. Chem. Sci.* **2024**, *15*, 8227.
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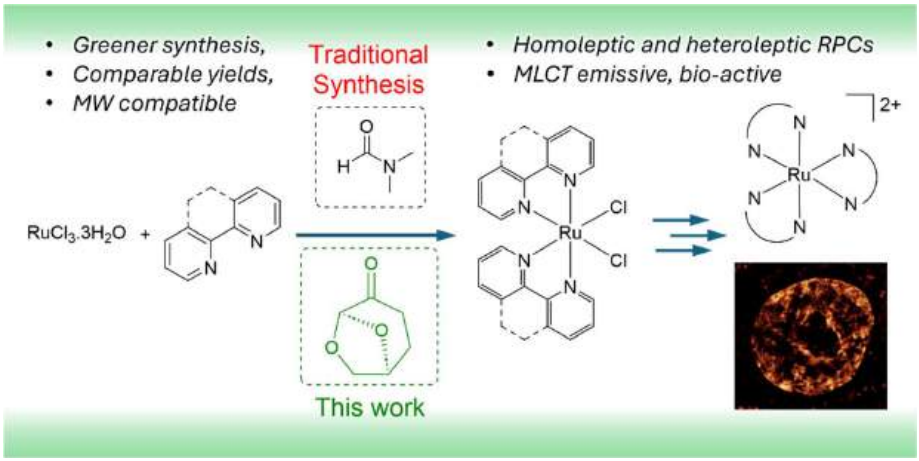
CBF - D3 - F07
Green(er) synthesis of MLCT-emissive ruthenium(II) polypyridyl complexes

Martin R. Gill[1]
[1]*Swansea University, UK*

Due to their flexible coordination chemistry, tuneable redox behaviour, stability in aqueous media, ability to emit from long-lived MLCT (metal to ligand charge-transfer) states, and capacity to bind biological targets with high selectivity, ruthenium(II) polypyridyl complexes (RPCs) find widespread use as luminescent probes and emerging bio-therapeutic agents.[1-3] Their versatility underpins a diverse range of applications including photocatalysis, light-harvesting, molecular and cellular imaging, and anticancer therapy.
Conventional synthetic routes to RPCs rely heavily on N,N′-dimethylformamide (DMF), a dipolar aprotic solvent designated a Substance of Very High Concern (SVHC) under EU REACH legislation. Its use presents a major obstacle to sustainable, large-scale production in compliance with the twelve principles of green chemistry. Here, we report a microwave-assisted, two-step synthesis employing Cyrene™ (dihydrolevoglucosenone), a biorenewable cellulose-derived solvent, as a direct and effective substitute for DMF in both the preparation of the key cis-$Ru(N\hat{}N)_2Cl_2$ precursor complexes and the subsequent formation of homoleptic $[Ru(N\hat{}N)_3]^{2+}$ type complexes (including the benchmark luminophore $[Ru(bpy)_3]^{2+}$) and heteroleptic $[Ru(N\hat{}N)_2(N'N')]^{2+}$ type complexes. Two novel methylated intercalators, $[Ru(bpy)_2(10,11\text{-dmdppz})]^{2+}$ and $[Ru(5,5'\text{-dmbpy})_2(10,11\text{-dmdppz})]^{2+}$, were synthesised using this route. Both exhibited exceptionally high DNA-binding affinities and pronounced MLCT luminescence enhancement upon intercalation, moderate cytotoxicity towards cancer cell lines and compatibility with advanced imaging techniques such as STED microscopy.[4]
Placed in the context of the sustainable manufacture of metallodrugs and imaging agents, challenges of extending this approach to hydrophobic ligand systems, solvent lifecycle, and promoting broader adoption of green synthetic practices in coordination and organometallic chemistry will be discussed.



We thank the Royal Society of Chemistry for funding.

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[2]Gill, M. R. *et al*., *Angew. Chem. Int. Ed.* **2022**, *61*, e202117449
[3]Elgar, C. E. *et al. J. Am. Chem. Soc.* **2023**, *145*, 1236-1246.
[4]James, S. J. *et al*. *Dalton Trans*. **2024**, *53,* 18506-18514.

CBF - D4 - O01
Pharmacological modulation of human immunity: A chemistry-based approach

Francesco Peri[1], Alessio Romerio[1], Federico Lami[1], Monsoor Mohammed Shaik[1], Alice Italia[1], Sonsoles Martin-Santamaria[2], Giovanna D'Amico[3], Sara Lovisa[4]
[1]Dept. of Biotechnology and Biosciences, University of Milano-Bicocca, Italy; [2]Centro de Investigaciones Biológicas Margarita Salas CSIC, Spain; [3]Dept. of Biomedical Sciences, Humanitas University, Italy; [3]Unità di Immunologia e Terapia Cellulare Fondazione Tettamanti, IRCCS San Gerardo dei Tintori, Italy

Toll-Like Receptor 4 (TLR4) is a fundamental switch of innate immunity. It can be activated by pathogen-associated ligands (mainly bacterial lipopolysaccharide, LPS) and by endogenous danger-associated molecules. TLR4 activation and signalling leads to cytokine production, inflammation, and innate immunity activation. Excessive TLR4 activation causes sepsis and acute and chronic inflammatory pathologies, TLR4 antagonists are therefore candidates as anti-inflammatory agents, while compounds that stimulate TLR4 are potential vaccine adjuvants and immunotherapeutics. We developed a technological platform based on innovative, synthetic, small molecular TLR4 agonists and antagonists that are able to selectively activate and inhibit TLR4. Interestingly, our agonists could differentially act on different TLR4-initiated pathways (MyD88 and/or TRAM/TRIF) thus allowing the dissection of the different pathway-associated functions.[1] Our molecules are not only interesting chemical biology tools to interrogate innate immunity, some antagonists are in preclinical development phase as anti-inflammatory drugs to treat acute and chronic inflammations, such as influenza virus-induced acute lung inflammation (ALI) and cytokine storm[2], inflammatory bowel diseases (IBDs)[3], vascular inflammation, atherosclerosis, neuroinflammation[4] and fibrosis. Synthetic TLR4 agonists developed by our group[5] and mimicking the activity of monophosphoryl lipid A (MPLA) are in preclinical development as vaccine adjuvants and cancer immunotherapeutics.

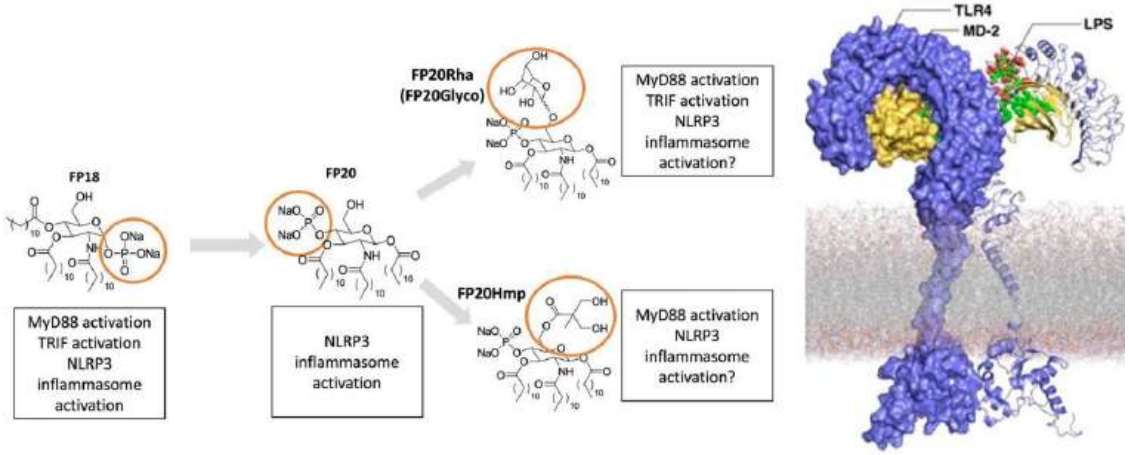

Fig. Left: Several generations of glucosamine-basedTLR4 agonists developed by our group and their specific activity on TLR4 pathways. Right: the activated TLR4/MD-2 dimeric complex

In this lecture new generations of TLR4 modulators will be presented together with SAR studies. The investigation of the mechanism of action of these small molecules, allows to understand the relation among their chemical structure and the activation or the inhibition of different molecular circuits linked to cancer and fibrotic diseases.

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[3]Facchini F.A.; Peri, F. et al. *Eur. J. Of Clin. Pharmacol.* **2020**, 76, 409–418
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CBF - D4 - O02
Environmental pollution and asthma: EXPOSOMIC approach

Chiara Maccari[1,2], Paola Mozzoni[1,2], Silvana Pinelli[1], Valentina Fainardi[4], Matteo Malvezzi[3], Stefano Renzetti[3], Massimo Corradi[1,2], Silvia Ranzieri[1,2], Roberta Andreoli[1,2]
[1]Laboratory of Industrial Toxicology and Advanced Analytical Methods, Dept. of Medicine and Surgery, University of Parma, Italy; [2]Center of Excellence for Toxicological Research (CERT), University of Parma, Italy [3]Dept. of Medicine and Surgery, laboratory of biostatistic, University of Parma, Italy; [4]Dept. of Medicine and Surgery, Clinic of Pediatrics, Pietro Barilla Children's Hospital, University of Parma, Italy

Asthma is among the most prevalent chronic respiratory diseases worldwide, and increasing evidence suggests that exposure to air pollutants contributes to disease severity and progression. In this study, an integrated analytical approach combining gas chromatography/mass spectrometry (GC–MS) and liquid chromatography tandem mass spectrometry (LC–MS/MS) was applied to investigate the relationship between environmental exposure, oxidative stress, and inflammation within an exposomic framework [1]. Spot urine samples were collected from 450 subjects living in Parma (Italy), including healthy individuals (200 adults and 100 children) and asthmatic patients (100 adults and 50 children). Urinary biomarkers of exposure to benzene, toluene, ethylbenzene, and xylenes (BTEX), styrene, and methyl tert-butyl ether (MTBE) were quantified by GC–MS following solid-phase microextraction (SPME). Biomarkers of oxidative nucleic acid damage were quantified by LC–MS/MS using an ExionLC system coupled to a QTRAP 6500+ mass spectrometer, while urinary HMGB1 was measured by ELISA. Asthmatic adults exhibited significantly higher urinary BTEX concentrations compared with healthy controls, accompanied by increased levels of oxidative DNA damage markers, including 8-oxo-7,8-dihydro-2′-deoxyguanosine (8-oxo-dG), and the epigenetic marker 5-methylcytosine (5MeCyt). The combined visualization of exposure and effect biomarkers highlights a systematic shift toward higher oxidative stress and epigenetic alteration in asthmatic subjects, demonstrating the capability of integrated mass spectrometric techniques to capture complex exposure–response relationships within an exposomic framework [2]. Overall, this work emphasizes the central role of advanced analytical chemistry in integrating environmental and biological measurements, providing mechanistic insight into pollutant-related respiratory diseases and reinforcing the interdisciplinary interface between chemistry, environment, and human health.

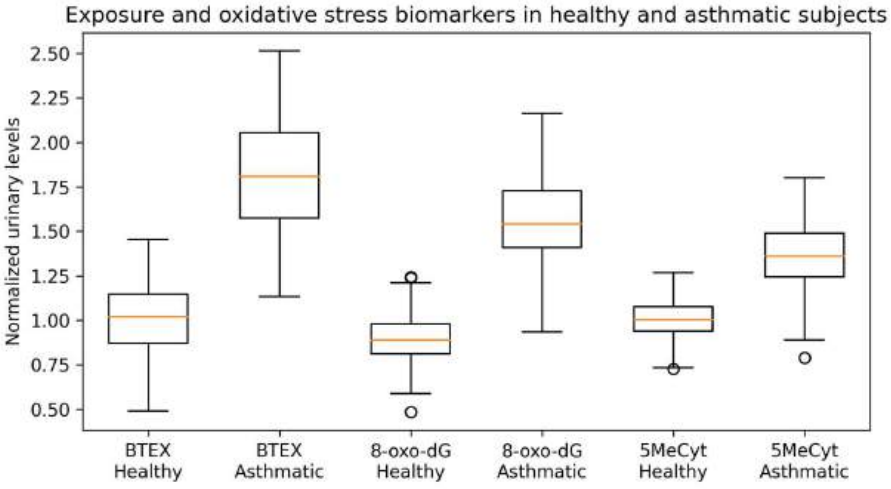

Fig. 1. Combined box plot of urinary exposure and effect biomarkers in healthy and asthmatic subjects. BTEX concentrations and oxidative stress markers (8-oxo-7,8-dihydro-2′-deoxyguanosine, 8-oxo-dG, and 5-methylcytosine, 5MeCyt) are reported as normalized urinary levels. Asthmatic subjects show consistently higher values across all biomarkers.

[1]Abboud, M. M., Al-Rawashde, F. A., & Al-Zayadneh, E. M. (2022). J*ournal of Asthma*, 59(11).
[2]Bellou, V., Gogali, A., & Kostikas, K. (2022). n *Journal of Personalized Medicine* (Vol. 12, Issue 8)

CBF - D4 - O03

Phytochemical profiling and quantification of glucosinolates in radish microgreens and evaluation of their H_2S-mediated vasodilatory activity

Vincenzo Piccolo[1], Maria Maisto[1], Adua Marzocchi[1], Erika Esposito[1], Emma Mitidieri[1], Roberta d'Emmanuele di Villa Bianca[1], Gian Carlo Tenore[1]
[1]*Dept. of Pharmacy, University of Naples Federico II, Italy.*

Microgreens are increasingly recognized as sustainable plant-based biofactories for the standardized production of high-value phytochemicals. Among Brassicaceae, radish (*Raphanus sativus* L.) microgreens are characterized by a complex glucosinolate (GSL) profile. In this study, an integrated chemical, analytical, and functional approach was applied to identify glucosinolate-rich radish microgreens through cultivar and growth-condition screening under controlled hydroponic cultivation. Six *Raphanus sativus* L. cultivars (Red Rubin, Daikon, Saxa, White Tips, China Rose, and Tango) were harvested at different developmental stages. Lyophilized microgreens were extracted using food-grade aqueous or hydroalcoholic protocols and analyzed by HPLC-HESI-MS/MS. A rapid precursor ion scan strategy targeting the diagnostic sulfate fragment (*m/z* 97) was developed for selective screening of intact GSLs. Several GSLs were identified, including glucoraphasatin, glucoraphenin, glucoraphanin, glucobrassicin, and sinapoylated and benzoylated derivatives. Targeted quantification by Multiple Reaction Monitoring acquisition mode revealed that cv. Saxa exhibited the highest total GSL content, reaching approximately 100 mg/g dry weight (DW) at the optimal harvesting time. In parallel, total polyphenols, anthocyanins, and antioxidant capacity were determined by spectrophotometric assays (DPPH, ABTS, FRAP). Cv. Tango microgreens showed a balanced phytochemical profile, combining high total GSLs with elevated polyphenol content (17.21 ± 0.67 mg GAE/g DW) and anthocyanins (11.91 ± 0.02 mg cyanidin-3-glucoside equivalents/g DW), together with strong antioxidant activity (DPPH IC_{50} = 0.67 mg/mL). Therefore, Tango microgreens were selected for functional assays. Their aqueous extracts induced concentration-dependent hydrogen sulfide (H_2S) release (up to 30 μM in cell-free conditions) and produced significant relaxation of pre-contracted vascular rat rings by an *ex vivo* experiment. Overall, this work establishes a robust chemical framework for the selection and standardization of glucosinolate-rich radish microgreens as promising nutraceuticals targeting vascular health.

[1]Demir, K. et al., *Food Chemistry*. **2023**, *401*, 134088.
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CBF - D4 - O04
Synthetic gene networks for tunable regulation of enzyme-inhibitor complexes

Giorgia Gambardella[1], Francesco Grassi[1], Simona Ranallo[1]
[1]Dept. of Chemical Science and Technologies, University of Rome Tor Vergata, Rome, Italy

Precise control of biomolecular interactions is central to synthetic biology, therapeutics, and biosensing[1]. Enzyme-inhibitor complexes, in particular, represent a powerful but underutilized axis for programmable regulation of enzymatic activity due to their inherent reversibility and specificity. However, conventional approaches to modulate these enzyme-inhibitor interactions often lack dynamic tunability and contextual responsiveness. Here, we present a modular platform that harnesses the programmability of synthetic nucleic acids and the versatility of cell-free gene networks to dynamically regulate enzyme-inhibitor complexes. Specifically, synthetic gene circuits are engineered to respond to specific targets and trigger the transcription of functional RNA strands in a highly programmable and orthogonal manner. The so transcribed RNA strands act as regulatory elements for the modulation of enzyme-inhibitor interactions. By encoding these logic-driven responses in transcriptional modules, we achieved repression or activation of the enzymatic activity, thus demonstrating how transcriptionally encoded RNA regulators can be used to achieve input-specific and dose-responsive control in a tunable and reversible way (Figure 1). We demonstrate this using two different enzyme-inhibitor systems. Specifically, the first couple comprised alpha amylase, a well-known enzyme with broad industrial applications[2], and its inhibitor derived from *Triticum aestivum*. The second system involves the elastase and the α1-antitrypsin as inhibitor responsible for counteracting the potential cellular damage mediated by elastase[3]. Our platform offers a new route to achieve a dynamic biochemical control with broad implications for therapeutic enzyme regulation, biosensing and synthetic biology.

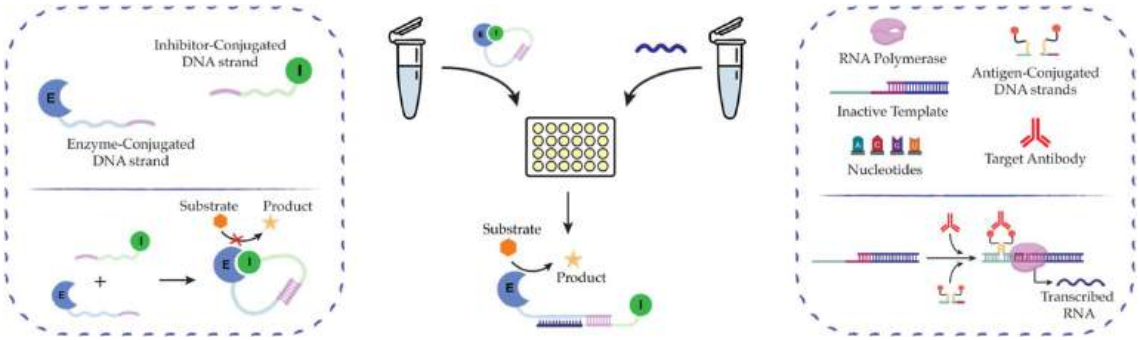

Fig. 1. Representative scheme of the platform. (Left) Two proteins conjugated to two different DNA strands with a complementary region (in purple). (Right) The gene network which involves a pair of antigen-conjugated DNA strands designed to hybridize to the single-stranded portion of a synthetic DNA template and reconstitute the incomplete T7 RNA Polymerase promoter domain only upon recognition of a specific target antibody. The transcribed RNA will be able to remove the inhibitor from the enzyme through base pair interactions thus letting the conversion from substrate to product occur.

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CBF - D4 - O05

Plasma-functionalized electrospun PLA–PCL Scaffolds implanted in rabbits for articular cartilage regeneration

Roberto Olayo-Gonzalez[1], Nancy C. Islas-Arteaga, Omar E. Uribe-Juárez[2], Maria G. Flores Sanchez[2]
[1]Dept. of Physics, Metropolitan Autonomous University, Mexico; [2]University La Salle, Mexico

Articular cartilage is a specialized connective tissue that covers the surfaces of synovial joints, providing a smooth, low-friction surface with high resistance to wear. However, due to its avascular nature, its regenerative capacity after injury is limited. Damage to articular cartilage can lead to pain, loss of mobility, and the development of degenerative joint diseases such as osteoarthritis. To address this challenge, tissue engineering has proposed several strategies for cartilage repair, including cell-based therapies, the use of growth factors, biomolecules such as aggrecans, and the development of biomaterials.

In this work, electrospun PLA–PCL biomaterials functionalized with polypyrrole (PPy) via plasma polymerization were developed[1] and evaluated as a potential treatment for cartilage regeneration in a rabbit animal model, through implantation in the knee joint, in combination with chondrocytes and the aggrecan protein.

The neocartilages obtained from the different materials were evaluated through histological analyses, and their mechanical behavior was modeled using a generalized Maxwell model with nonlinear contributions, which converges to two effective parameters: the storage modulus and the dissipation modulus. Materials implanted without chondrocytes and aggrecans led to the formation of fibrous cartilage with discontinuous integration with the subchondral bone. In contrast, the material combined with aggrecan, and chondrocytes showed mature and continuous integration with the subchondral bone, as well as a zonal structure like that of native cartilage. The mechanical response of the neocartilages was described using a nonlinear generalized Maxwell model. The parameters obtained for the different neocartilages were of the same order of magnitude, with uncertainties below 6%.

[1] Islas-Arteaga, N. *Int. J. Polym. Mater. Polym. Biomater.*. **2019**, 68,18, 1089–1098.

CBF - D4 - O06
Tunable biopolymer production from CO_2 through biotechnological processes

Heleen De Wever[1], Wouter Van Hecke[1]
[1]Flemish Institute for Technological Research (VITO), Belgium

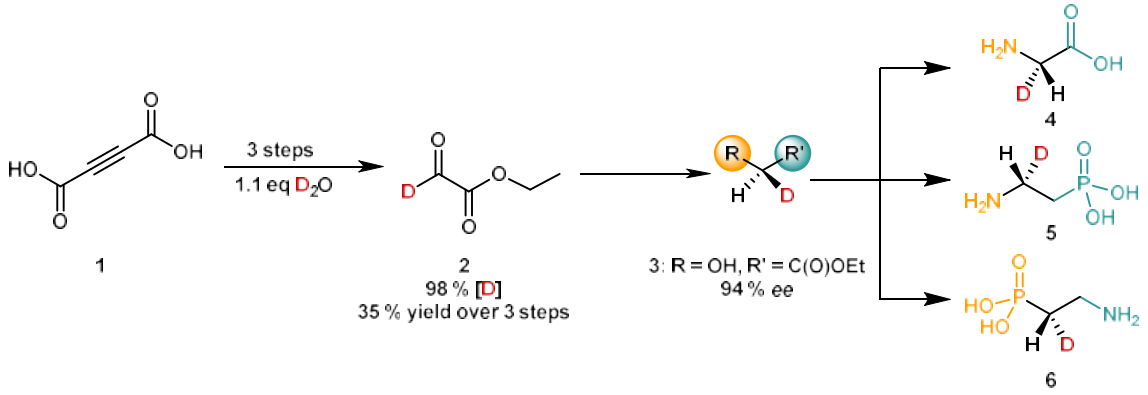
Nowadays it is recognized that rather than just storing it, emitted CO_2 can be a valuable source of carbon for the production of commercially valuable products. In this presentation we will focus on the use of CO_2 as feedstock for the synthesis of biopolymers using biotechnology.
First we will discuss the sustainable production of the biopolymer polyhydroxyalkanoate (PHA) from CO_2. VITO developed an innovative alternative fermentation strategy using organic and inorganic waste streams as feedstocks for the biomass growth and PHA production phase respectively. Test work encompassed optimizations with mock-up gas mixtures and real CO_2-containing off-gases. Moreover, PHA characteristics were compared with and similar to the properties of commercial PHA samples produced from organic substrates.
PHA are interesting materials because they can be tailored to meet the product specifications of end users. As a first, VITO successfully produced the copolymer poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV), under combined supply of CO_2 and valeric acid.
The indirect conversion of acetic acid from CO_2 into PHA is an interesting alternative for the direct production of PHA from CO_2 in terms of CO_2 fixation, H_2 consumption, substrate cost, safety and process performance. A cultivation method using acetic acid was therefore developed and a proof-of-concept provided for the synthesis of Polyhydroxybutyrate (PHB) and PHBV.
Alternative hybrid abiotic/biotic concepts can avoid or reduce gas solubility issues. A well-known example is renewable methanol production combined with methanol fermentation. We developed and intensified a bioprocess using *Methylorubrum extorquens* for the production of microbial proteins and PHA and reported for the first time PHBV production on methanol-pentanol mixtures at bioreactor scale.
Interestingly, microbial proteins and PHA can also be jointly produced in microbial biomass, co-extracted and co-valorized for novel bioplastics application. We therefore finetuned their combined production and studied their joint or separate downstream processing.

The authors gratefully acknowledge Flemish Science Foundation FWO for funding the PROMIPOL project (European Union – NextGenerationEU, Contract G0G3922N).

CBF - D4 - O07
Small stereoselectively deuterated molecules at the chemistry–biology interface

Sebastian-Felix Fritz[1,2], Hannah Riedmüller[1], Katharina Pallitsch[1]
[1]Institute of Organic Chemistry, University of Vienna, Vienna; [2]Doctoral School in Chemistry, University of Vienna, Vienna

Small molecules with high enantioisotopic purity are essential substrates for mechanistic studies in chemical biology, particularly for elucidating enzyme-catalysed transformations and stereospecific interactions. However, generalisable methods for their synthesis, as well as reliable strategies for the determination of their absolute configuration, remain limited. [1–4]
In our work, we report the efficient synthesis of key synthetic intermediate **2** and a robust, reproducible reaction sequence that enables the efficient preparation of enantioisotopically enriched substrates from **2**. The developed purely chemical method provides a versatile toolkit for the synthesis of a variety of enzyme substrates which are typically only accessible by the use of chemoenzymatic syntheses.



The key intermediate **3** was efficiently converted into a structurally diverse set of isotopically labelled synthons via stereospecific S_N2 reactions, preserving enantiopurity throughout the entire reaction sequence. This modular approach enables the rapid and (atom) economic assembly of chemically and biologically relevant building blocks, thereby broadening the synthetic scope and utility of isotopically labelled probes in chemical biology. The resulting compounds might serve as tools for investigating enzyme mechanisms, metabolic flux rates, and molecular recognition events alike.

Acknowledgements: This research was funded in whole or in part by the Austrian Science Fund (FWF) [10.55776/PAT2590124]. This project is embedded in the Doctoral School of Chemistry at the University of Vienna.

[1]Sonstrom, R. E., *et al*. Rapid *Organic process research & development* **2023**, *27*, 1185–1197
[2]Rowbotham, J. S., *et al. Nature communications* **2020**, *11*, 1454
[3]Kopf, S. *et al. Chemical reviews* **2022**, *122*, 6634–6718
[4]Mills, M. *et al. Angewandte Chemie (International ed. in English)* **2022**, *61*

CBF - D4 - O08

Plant-derived extracellular vesicles from grape pomace as bioactive nanocarriers for anti-aging nutraceutical applications

Maria Maisto[1], Vincenzo Piccolo[1], Marlo De Vivo[1], Serena Sagliocchi[2], Monica Dentice[2], Gian Carlo Tenore[1]
[1]Dept. of Pharmacy, University of Naples Federico II, Italy; [2]Dept. of Clinical Medicine and Surgery, University of Naples Federico II, Italy

The progressive increase in life expectancy has intensified the need for innovative and sustainable strategies to counteract age-related functional decline. In this context, plant-derived extracellular vesicles (EVs) have emerged as promising bioactive nanocarriers for anti-aging nutraceutical applications. EVs are cell-derived nanoscale particles bounded by a phospholipid bilayer and secreted as physiological mediators of intercellular communication. They encapsulate bioactive lipids, plant secondary metabolites, and regulatory nucleic acids, acting as a naturally protected delivery system. Accordingly, the primary objective of the present project is to isolate EV-enriched complexes from a sustainable food waste source, specifically the grape pomace of *Vitis vinifera* L. cv. Aglianico, to develop an EVs-based nutraceutical formulation with potential anti-aging activity.
Lyophilized grape pomace was treated in RNase-free water at a 1:5 (w/v) ratio and subjected to differential centrifugation at 650 × *g*, 3000 × *g*, and 10,000 × *g*. The resulting supernatant was sequentially ultracentrifuged at 135,000 × *g* for 2 h and 110,000 × *g* for 40 min. The final pellet was resuspended in RNase-free water. Particle concentration, size distribution, and morphology were determined by Tunable Resistive Pulse Sensing (TRPS), revealing a mean diameter of 148 ± 68.4 nm and a concentration of 1.55 × 10^{10} particles/mL. The chemical composition was investigated using an integrated LC–MS/MS approach, enabling the identification of more than 20 secondary metabolites as well as comprehensive proteomic and lipidomic profiles of the isolated EVs complexes.
The anti-aging potential of the isolated EV complexes was evaluated in C2C12 myoblasts, focusing on the AMPK–FOXO3 signaling axis, a key regulator of aging-related pathways. EVs-treatment for 48 h resulted in a significant increase in AMPK and FOXO3 expression levels compared to control, with a 20% and 60% upregulation, respectively ($p < 0.005$), accompanied by a modulation of phosphorylation states pFOXO3/FOXO3 and pAMPK/AMPK**.**

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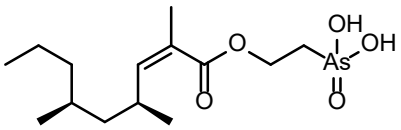
CBF - D4 - O09
Total synthesis of Bisenarsan - An organo-arsenic metabolite from Streptomyces

Ihor Kholomieiev, Jeya Prathap Kaniraj, Adriaan J. Minnaard
Stratingh Institute for Chemistry, University of Groningen, The Netherlands

The first synthesis of Bisenarsan will be presented, together with the determination of its absolute configuration by preparing both enantiomers and comparing these to the natural isolate.
In 2023, Hoshino and Onaka *et al*.[1] isolated Bisenarsan from *Streptomyces lividans.* This marked the first arsenic containing secondary metabolite isolated from Actinomycetes, and a major discovery in biosynthesis as the unprecedented 2-hydroxyethyl arsonic acid fragment originates from arsenoenolpyruvate. The discovery provides a new perspective on the presence and function of organo-arsenic natural products, that extends beyond the established detoxification mechanisms, organisms use to survive in arsenic-rich environments. Bisenarsan possibly acts as a protoxin, used by streptomyces to secure an ecological niche.
The levels of organo-arsenic compounds in bacteria are low, and bisenarsan is difficult to isolate. To study its structure and behaviour, chemical synthesis is therefore instrumental. However, the chemistry of organo-arsenic compounds, in particular in natural product synthesis, is hardly developed. Therefore, we set out to prepare bisenarsan and contribute to synthesis strategies[2] and methods in this field.



Bisenarsan, an organo-arsenic compound from *Streptomyces*

[1]Hoshino, S.; Ijichi, S.; Asamizu, S.; Onaka, H. *J. Am. Chem. Soc*. **2023**, *145*, 17863–17871.
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CBF - D4 - O10
Transcriptional circuits control of Hybridization Chain Reaction (HCR)

Cecilia Scandurra[1], Simona Ranallo[1]
[1]Dept. of Chemical Science and Technologies, University of Rome Tor Vergata, Rome, Italy

In recent decades, advances in synthetic biology have enabled the transition from cell-based to cell-free biosensors, significantly expanding their application range from environmental monitoring[1] to medical diagnostics[2]. Indeed, cell-free biosensors are emerging as cost-effective and user-friendly platforms for the detection of viral nucleic acids[3] and small molecules[4]. By coupling the programmability of synthetic nucleic acids with the high sensitivity and specificity of cell-free systems, our group recently reported the first examples of cell-free biosensors for antibodies detection[5] that exploit the use of synthetic antigen-conjugated DNA strands. However, improving the sensitivity of such platforms remains a major challenge. Despite several strategies have been reported so far to address this limitation, those all include the use of enzymes[6]. Here, we propose to combine the features of DNA nanotechnology with those of cell-free system to develop an enzyme-free amplification strategy for the ultrasensitive detection of different biomarkers. Specifically, we developed a cell-free circuit that couples the molecular recognition of programmable antigen-conjugated synthetic nucleic acids and genetic circuits with the robust, enzyme-free amplification capabilities of Hybridization Chain Reaction (HCR)[7], enabling the ultrasensitive, specific and selective detection of different biomarkers, including three clinically-relevant antibodies (i.e., anti-HIV, anti-MUC1 and Cetuximab antibodies).

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CBF – D4 – O11

Synthesis & structure-activity relationship study on a plant-derived glycoside that attenuates virulence in *Pseudomonas aeruginosa*

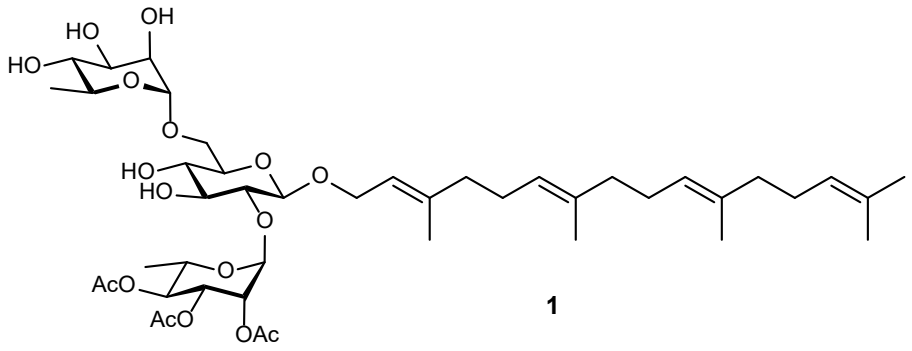
Haris Majstorović[1], Xiaohua Jiang[1], Arnaud Cudré-Mauroux[1], Carmen R. Cori[1], Fabricio Ramírez Cortés[1], Han-Yi Huang[2], Alexandre Persat[2], Rachel Hevey*[1]

[1]Molecular Pharmacy, Dept. Pharmaceutical Sciences, University of Basel, Switzerland; [2]Global Health Institute & Institute of Bioengineering, School of Life Sciences, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Pseudomonas aeruginosa is a significant cause of hospital-acquired infections, and in particular poses a severe threat to individuals with cystic fibrosis or compromised immune systems.[1] Its capacity to rapidly develop resistance to antimicrobial drugs has led the World Health Organization to classify it as a pathogen urgently requiring new therapeutic strategies.[2]

During a recent screening campaign of a natural product library, glycoside **1** was observed to attenuate *P. aeruginosa* virulence. To enable a detailed structure–activity relationship study, we developed methodology for the total synthesis of glycoside **1** together with a series of structurally related analogues. This natural product, originally isolated from the plant *Dalbergia oliveri*, is composed of a trisaccharide core linked to a geranylgeraniol-derived diterpenoid aglycone. Synthesis of the compound library presented several challenges, particularly in appending the diterpenoid aglycone and developing an approach for regioselective glycosylation of the different rhamnose residues. Nevertheless, we successfully developed a synthetic route to this complex molecule and its analogues, and with collaborators have been assessing their biological activities to establish well-defined structure-activity relationships.

Acknowledgments: Project supported by the Swiss National Science Foundation (320030-231409) and the University of Basel.



1

Fig. 1. Structure of plant-derived glycoside **1**.

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CBF - D4 - F01
Design and synthesis of lipid substrates for sterol imaging

Mihai-Alexandru Molența[1], Anamaria Hanganu[1,2], Augustin M. Mădălan[1], Codruța C. Popescu[1], Mihaela Matache[1,3], Adrian Șalic[1,4]
[1]University of Bucharest, Faculty of Chemistry, Dept. of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Research Centre of Applied Organic Chemistry, Romania; [2]"Costin D. Nenitzescu" Institute of Organic and Supramolecular Chemistry of the Romanian Academy; [3]University of Bucharest, Faculty of Interdisciplinary Sciences, Dept. of Interdisciplinary Sciences, Romania; [4]Harvard Medical School, Dept; of Cell Biology, USA

Alteration of lipid structure, function, or dysregulation of lipid metabolism are factors implicated in the pathology of a large number of diseases, including cardiovascular and neurodegenerative diseases. The way in which the distribution of lipids specific to organelles is established and maintained is only partially understood, for example, kinetics of intracellular transport or local metabolism. To date, methods for high-resolution microscopic visualization of lipids in vivo are underdeveloped [1].
Cholesterol plays a critical role in normal cellular physiology by regulating the fluidity and permeability of cell membranes [2]. Current methods for visualizing its processes include, among others, intrinsically fluorescent sterols or their functionalization with fluorogenic moieties. All of these have disadvantages such as low quantum yields, high cytotoxicity, or incompatibility due to extensive functionalization [3].
Sterol analogs functionalized with alkyne groups are efficiently incorporated into cell membranes and can be conveniently visualized by high-resolution microscopy using CuAAC click reactions with azide-containing fluorophores. Their use has been demonstrated for visualization of the subcellular distribution of cholesterol and detection of sterols and choline phospholipids by two-color microscopy [3].
In this work, we present synthesis and characterization of cholesterol-derived fatty acid esters functionalized with alkyne or azide groups for visualization in cells by fluorescence microscopy.

Acknowledgements: This work was carried out with the financial support of the National Research Agency, PNRR/2022/C9/MCID/I8, CF 760056/23.05.2023, cod 235/29.11.2022.

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CBF - D4 - F02
Synthesis and characterization of novel rhodamine and coumarin-based fluorophores

Magdi El Fergani[1], Bogdan-C. Enache[1,2], Mihai-Alexandru Molenţa[1], Anamaria Hanganu[1,3], Codruţa C. Popescu[1], Adrian Salic[1,4], Mihaela Matache[1,5]
[1]University of Bucharest, Faculty of Chemistry, Dept. of Inorganic, Organic Chemistry, Biochemistry and Catalysis, Research Centre of Applied Organic Chemistry, Romania;[2]SC Microsin SRL, Dept. of Research and Development, Romania; [3]Institute of Organic and Supramolecular Chemistry "C.D. Neniţescu" of the Romanian Academy, Romania; [4]Dept. of Cell Biology, Harvard Medical School, Boston, USA; [5]Faculty of Interdisciplinary Studies, Dept. of Interdisciplinary Studies, University of Bucharest, Romania

Fluorescence-based techniques play a crucial role in visualizing and studying molecular and cellular processes due to their key features such as high sensitivity, spatial resolution, and compatibility with advanced imaging methods. Therefore, the performance of fluorescent probes depends strongly on their photophysical properties particularly quantum yield and photostability, which are essential for reliable imaging and sensing applications. Recent advances in chemical biology, modern microscopy and spectroscopy techniques, including confocal, multiphoton, and time-resolved fluorescence imaging, have extended their utility from basic chemistry to live-cell biology[1]. As example, two important classes of fluorophores in chemical biology are rhodamines and coumarins based compounds. Rhodamine dyes belong to the family of xanthene fluorophores, and structural modifications of this scaffold have led to the development of Si–rhodamines, in which replacement of the bridging oxygen atom with silicon significantly enhances the fluorophore efficiency. These fluorophores can be readily functionalized with bioorthogonal groups such as azides or alkynes, enabling site-specific labeling of biomolecules including proteins, nucleic acids, and nanomaterials via click chemistry[2]. In parallel, coumarin derivatives bearing similar clickable functionalities represent a complementary class of fluorescent probes with broad applicability in chemical biology and fluorescence imaging[3].
Based on this, our work presents findings on the synthesis and characterization (NMR and MS) of novel rhodamine and coumarin-based fluorophores.

Acknowledgements: Romanian Ministry of Research, Innovation and Digitization, PNRR/2022/C9/MCID/I8, nr. 760056/23.05.2023.

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CBF - D4 - F03

De novo analytical chemistry approaches for collagen and polyphenol characterization in Physalia physalis

Inês Ferreira[1,2], Amélia Rauter[1], Nuno Xavier[3], Andreia Silva[3], Carla Pires[2], Narcisa Bandarra[2]
[1]Centro de Química Estrutural, Institute of Molecular Sciences, CienciasULisboa, Portugal; [2]Division of Aquaculture, Upgrading and Bioprospecting, IPMA, Portugal; [3]Faculdade de Farmácia, Universidade de Lisboa, Portugal

Physalia physalis (Portuguese man o' war) is a gelatinous marine organism that remains largely unexplored from a chemical perspective, despite its structural complexity and ecological abundance [1]. An integrated chemical characterization of *P. physalis* was performed, focusing on collagen extraction and polyphenol profiling.

Using methodologies adapted from other jellyfish species [2,3], collagen was extracted from the pneumatophore via a pepsin-solubilization strategy, as conventional extraction methods proved ineffective due to the highly cross-linked nature of the tissue. Structural characterization by SDS-PAGE and FTIR spectroscopy confirmed the presence of type I collagen with preserved triple-helical integrity (Figure 1). To the best of our knowledge, this represents the first report of collagen extraction and structural characterization from *P. physalis*.

In parallel, the chemical profiling of tentacle-derived polyphenols was investigated. Owing to the absence of reference metabolomic data for *P. physalis* and related Hydrozoa, a de novo analytical workflow was required. High-resolution LC–MS/HRMS combined with MS/MS fragmentation enabled the identification of several phenolic compounds using authentic standards, while the elucidation of additional compounds is ongoing due to matrix complexity and limited database coverage.

Overall, this work highlights the value of advanced analytical chemistry approaches for unlocking the chemical potential of understudied gelatinous marine organisms and establishes *P. physalis* as a promising source of marine-derived biomaterials and naturally occurring compounds with prospective biotechnological and biomedical applications.

Fig. 1. Pepsin-soluble collagen extracted from the pneumatophore of *Physalia physalis*, showing the homogeneous appearance of the isolated collagen prior to structural characterization.

Acknowledgments: The authors are grateful to Fundação para a Ciência e a Tecnologia (FCT) for the financial support to Centro de Química Estrutural (project UIDB/00100/2020), CIIMAR (UIDP/CVT/00276/2020), the project PTDC/SAUNUT/30455/2017 and the grant 2021.06108.BD.

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CBF - D4 - F05

PEGylation-driven remodeling of the protein corona on PLGA nanoparticles: Implications for macrophage recognition

Lucio Spinelli[1], Pasquale D'Anna[1], Elva Morretta[1], Chiara Cassiano[1], Virgilio Piccolo[1], Martina De Rosa[1], Rebecca Amico[1], Paola De Cicco[1], Diego Brancaccio[1], Claudia Conte[1], Angela Zampella[1], Fabiana Quaglia[1], Maria Chiara Monti[1]

[1]Dept. of Pharmacy, University of Naples Federico II, Naples, Italy

The life of nanoparticles (NPs) inside biological environments is characterized by the quick absorption of proteins arising the so-called Protein Corona (PC). The formation of the PC is a crucial step that defines the behaviour of NPs and their interaction with the immune system[1]. To understand how the surface chemical composition of NPs can influence the nature of the adsorbed proteins, a study was conducted on a small library of polymeric nanoparticles composed of a mixture of different ratios of PLGA and PEG-PLGA. Although the formulations contained varying quantities of loaded PEG, the surface levels were similar, exhibiting only minor variations.

NPs were isolated using an optimized microfiltration protocol that allows for a soft and thorough recovery of the NPs-Corona complexes. The LC-MSMS analysis revealed a distinct pattern of protein adsorption (Fig. 1), that changed along the composition of the NPs.

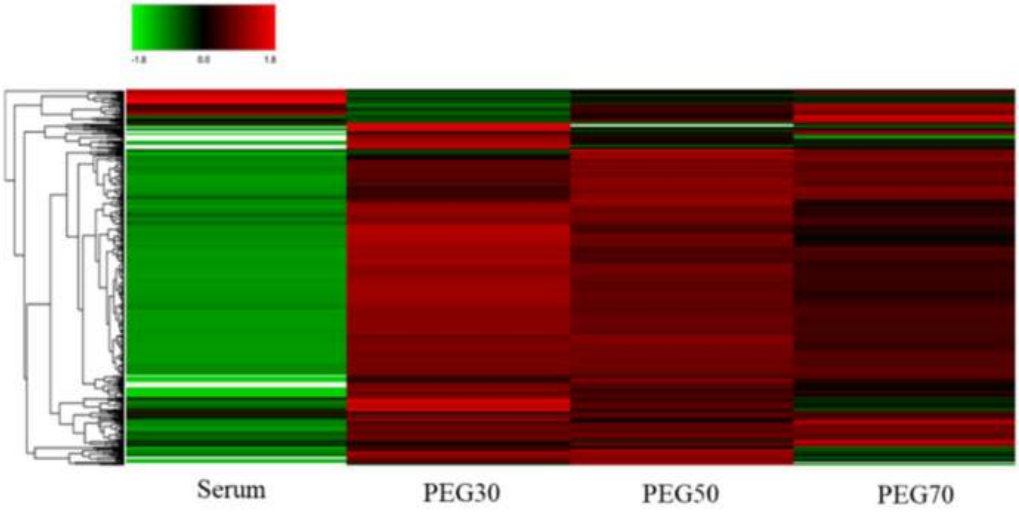

Fig. 1. Protein pattern in the different formulation visualized as a heatmap

Uptake studies in BMDMs were also conducted and resulted in a distinct inverse relationship between PEG quantity in the formulation and macrophage internalization. This data suggests that PEGilation does not hinder the protein adsorption itself[2] but rather influences the nature and abundance of the proteins that make the PC, supporting the hypothesis that an optimal opsonin/dysopsonin balance is essential for the internalization mechanism. These findings underscore the importance of rigorous surface characterization and PC profiling to predict and tune nanocarrier performance in vivo

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CBF - D4 - F08

Synergistic cancer therapy targeting LAG-3&PD-L1 through co-administration of flavonoid and durvalumab

Konrad Barnowski[1,2], Wen Zhang[3], Judyta Cielecka-Piontek[4], Łukasz Skalniak[1], Jacek Plewka[1]
[1]Faculty of Chemistry, Jagiellonian University, Poland; [2]Doctoral School of Exact and Natural Sciences, Jagiellonian University, Poland; [3]College of Pharmaceutical Science, Zhejiang University of Technology, China; [4]Faculty of Pharmacy, Poznan University of Medical Sciences, Poland

Cancer immunotherapy has changed the landscape of cancer treatment. By using inhibitors of immune checkpoint protein interactions, we reactivate the patient's immune system, enabling it to recognize and destroy cancer cells. The primary target in such therapy is unquestionably the PD-1/PD-L1 interactions, but new emerging proteins are also being considered. For example, blockage of LAG-3 protein interactions with its ligands – MHCII, and FGL1 – proved to also effectively reactivate T cells.

Current state-of-the-art cancer immunotherapy is 2022 FDA-approved synergistic anti-PD-L1 (nivolumab) and anti-LAG-3 (relatlimab) monoclonal antibodies therapeutic, used in the advanced melanoma. Current research is focused on proposing new, small molecule drugs, targeting those proteins. Although such compounds are well-developed in the case of PD-L1 protein, research on LAG-3/ligands interactions inhibitors is in the very beginning phase[1].

In this work, we propose synergistic cancer therapy through co-administration of durvalumab (anti-PD-L1 drug) and a flavonoid. Herein we confirmed direct binding of this molecule to LAG-3 (MST, K_D=4.6 μM) and its blockade of LAG-3/MHCII interactions (HTRF, IC_{50}=19.3 μM), proofing its immunotherapeutic mechanism. We also overcame flavonoid limitations of low aqueous and lipid solubility, by preparing the polymer-based formulation. Such a flavonoid formulation, co-administered with durvalumab, proved to be effective *in vivo* (hPD-L1-MC38 colon cancer tumor model in C57BL/6 mice), reducing tumor weight better than any constituent alone (**Figure**).

Our results provide first *in vivo* proof of synergistic action of anti-PD-L1 monoclonal antibody and small molecules targeting LAG-3/MHCII interactions. These findings open new avenues for developing cost-effective and potentially orally available addition to currently applied cancer immunotherapies.

The research was conducted as part of the OPUS grant “Innovative small molecule inhibitors targeting LAG-3 and the MHCII complex for cancer immunotherapy,” funded by the National Science Centre of Poland (agreement number UMO-2024/53/B/NZ7/02801).

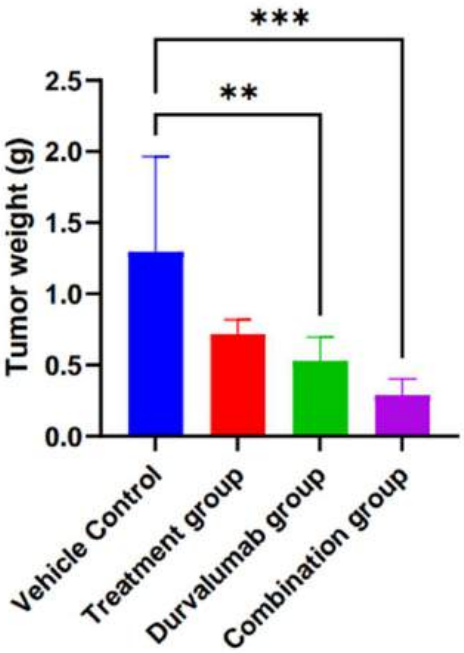

Fig. 1. Synergistic anticancer effect of co-administration of flavonoid and anti-PD-L1 antibody durvalumab on reducing murine tumor weight.

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The 10th EuChemS Chemistry Congress

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Catalyzing New Chemistry Solutions (CCS)

CCS - D1 - O01

Metal-driven structural rearrangement in Mn single-atom catalysts for selective photocatalytic oxidation of C–H bonds

Agustín de Arriba[1], Viktoria Velichko[1], Areti Moutsiou[1], Jesús López-Sánchez[2], Andrea Olivati[3], Annamaria Petrozza[3], Gianvito Vilé[1,*]

[1]Politecnico di Milano, Italy; [2]Instituto De Cerámica y Vidrio (ICV-CSIC), Spain; [3]Italian Institute of Technology, Italy

Visible-light-driven oxidation of C–H bonds to aldehydes using molecular oxygen is a key transformation for sustainable access to high-value intermediates in pharmaceuticals and fine chemicals.[1] In this contribution, we show that increasing the manganese (Mn) metal loading in single-atom catalysts based on carbon nitride triggers a metal-driven structural reorganization of the host framework, which fundamentally alters the nature of the Mn active sites and governs the photocatalytic oxidation of benzylic C–H bonds.

Comprehensive structural and spectroscopic characterization, including Raman spectroscopy (Fig.1A), X-ray absorption and photoelectron spectroscopies, together with aberration-corrected transmission electron microscopy (Fig.1B), confirms the atomically dispersed nature of manganese in all samples[2] and reveals that isolated Mn–N_x sites promote efficient charge separation and enable highly selective oxidation of benzylic substrates to the corresponding aldehydes. These Mn–N_x motifs are photocatalytic active (60% *p*-methoxytoluene conversion) and selective (54% yield to *p*-methoxybenzaldehyde) under visible-light irradiation (395 nm). In contrast, increasing the Mn loading above 1.0 wt.% induces a pronounced local reorganization of the carbon nitride framework into multilayered coordination motifs, leading to a complete loss of photocatalytic activity (Fig.1C). Complementary optical spectroscopy studies further confirm that higher Mn contents favor shorter photoinduced charge-carrier lifetimes, consistent with reduced charge-separation efficiency (Fig.1D).

Mechanistic investigations supported by density functional theory calculations indicate that isolated Mn sites mediate the activation of molecular oxygen to generate singlet oxygen and superoxide radical species, which drive the selective benzylic oxidation, while photogenerated holes contribute indirectly by sustaining continuous reactive oxygen species formation.[3] Finally, the optimized catalyst was successfully applied to ten different compounds and maintains high activity, stability, and selectivity under continuous-flow conditions.

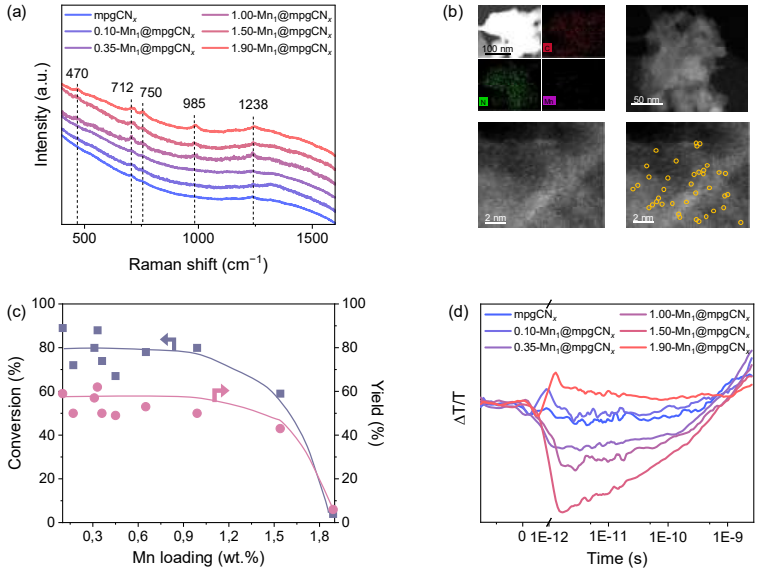

Fig. 1. (a) Raman spectra; (b) AC-TEM images at multiple magnifications with EDX mapping highlighting single Mn sites; (c) photocatalytic conversion and aldehyde selectivity; and (d) transient absorption spectra of catalysts with different Mn loadings.

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CCS - D1 - O02
Cu single atom catalyst for three component coupling reaction

Hushan Chand, Gianvito Vilé*
Dept. of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Italy

Single-atom catalysts (SACs) represent a new paradigm in heterogeneous catalysis, offering exceptional catalytic activity and selectivity.[1, 2] The design and development of SACs with site-specific and tunable catalytic properties remains a highly desirable yet challenging goal in catalysis.[3, 4] In this study, we have developed a single atom catalyst by anchoring copper single-atoms on a covalent organic framework (Cu@COF), for the efficient three-component A³ coupling reaction. The Cu atoms are atomically dispersed within the COF matrix through strong coordination with nitrogen sites, as confirmed by X-ray absorption spectroscopy and high-resolution electron microscopy. The catalyst showed excellent activity and selectivity in catalyzing the three-component A³ coupling reaction of amines, aldehydes, and alkynes, affording propargylamine derivatives in high yields. The Cu@COF catalyst exhibits excellent recyclability and stability and applicable to various substrates. The work demonstrates that rationally designed COF-supported Cu SACs can provide a robust and sustainable catalytic platform for multicomponent organic transformations.

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CCS - D1 - O03

Catalytic cross-coupling of *N*-terminal glycine C(sp^3)-H bonds in peptides enables rapid access to underexplored molecular space in drug discovery

Igor Beckers*[1,2], Anna-Carin Carlsson[1], Giovanna Mejia[3], Pernilla Korsgren[3], Vladimir P. Berishvili[1], Dirk De Vos[2], Magnus J. Johansson*[1]

[1]AstraZeneca, Dept. of Medicinal Chemistry, Discovery Sciences, BioPharmaceuticals R&D, Sweden; [2]KU Leuven, Dept. of Microbial and Molecular Systems, cMACS, Belgium; [3]AstraZeneca, Compound Synthesis and Management, Discovery Sciences, BioPharmaceuticals R&D, Sweden

The discovery of a new drug entails an enormous undertaking in which vast numbers of synthetic molecules are made and tested against a biological target of interest. Amide bond formations and Pd-catalyzed C-C cross-couplings are among the most frequently used chemical reactions in drug discovery. These generate vast combinatorial libraries of peptides and small molecules for high-throughput testing in bio-assays. While this strategy has proven highly successful in drug development, a long-standing question in the pursuit of future drug candidates is how to extend combinatorial cross-coupling chemistry to C(sp^3)-centers, with the aim to uncover poorly accessible three-dimensional molecular space. While impressive advances in cross-electrophile coupling, metallaphotoredox chemistry and oxidative radical couplings focus on bond formations with hydrophobic, flexible C(sp^3)-alkyl substituents, a late-stage C-C cross-coupling with backbone C(sp^3)-H bonds in peptides remained elusive so far. Because peptides play essential roles in biology and provide medicinal chemists with extensive libraries of building blocks, spanning a wide range of polarities, hydrogen bonding motifs and three-dimensional conformations, we have now developed a catalytic C-C cross-coupling methodology that selectively reacts on the C(sp^3)-H backbone in peptides at their *N*-terminal glycine residue. In the theme of “Catalyzing New Chemistry Solutions”, we reveal how fundamental insight in the C-C cross-coupling catalyzed its industrial implementation among AstraZeneca´s synthetic technologies for drug discovery. Supported by our mechanistic finding that cationic Pd-phosphine complexes can effectively trap otherwise reactive enolates formed from C(sp^3)-H bonds in peptides, studied via kinetic experiments, DFT-level computations and isotope labelling (Figure 1), the convergent cross-coupling was thoroughly benchmarked on a wide range of peptide sequences and generic drug molecules as late-stage functionalizations. We demonstrate application on modern synthetic platforms, including solid-phase peptide diversifications, macrocyclizations and high-throughput compound library synthesis (Figure 2). We evaluate their pharmacokinetic properties and discuss the newly accessed molecular space using cheminformatics.

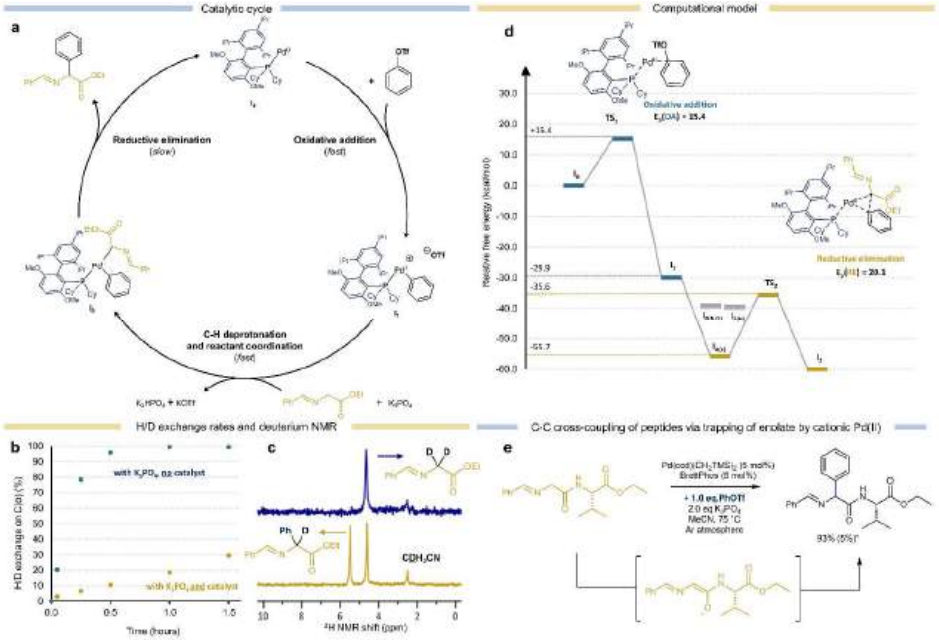

Fig. 1. Mechanistic investigation that supported our development of a catalytic system for the C-C cross-coupling of C(sp^3)-H bonds on *N*-terminal glycine residues in peptides. The underlying catalytic cycle (**a**) was investigated using H/D exchange kinetics (**b**), *in situ* NMR analysis of ^{2}H (**c**) and ^{13}C-labelled amino acid substrates and DFT-level modelling of the catalytic steps (**d**). The study revealed that reactive enolates formed from peptides are effectively trapped by a cationic Pd-Phosphine catalyst, enabling their selective C-C cross-coupling (**e**).

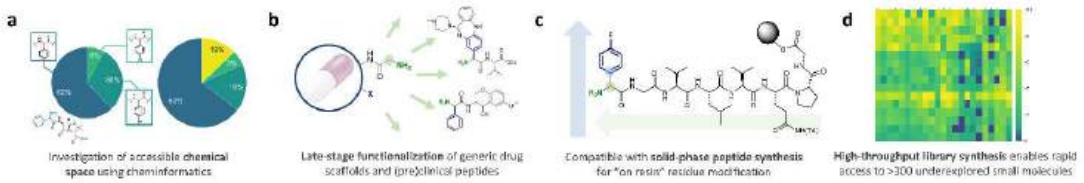

Fig. 2. Implementation of C(sp^3)-H cross-coupling of peptides on synthetic drug discovery platforms at AstraZeneca. Cheminformatics database analysis (**a**) highlights a lack of diversity in (hetero)aromatic C(α)-substituted amino acids among (pre)clinical compounds. Late-stage functionalizations of generic drug compounds of various therapeutic (**b**), and its application in solid-phase peptide synthesis (**c**) was demonstrated. The combinatorial cross-coupling was also applied in high-throughput compound library synthesis (**d**) to access underexplored a broad range of compounds with varying three-dimensional motifs and polarities for further testing of bio-activity and pharmacokinetic properties.

CCS - D1 - O04
1,1-Diaminoazine: A versatile organocatalyst

Kriti Mehta[1], Aabid Wani, P.V. Bharatam[1*]
[1]National Institute of Pharmaceutical Education and Research, S.A.S. Nagar, Punjab, India

Azines are 2,3-diaza analogues of 1,3-butadiene and are sometimes also referred as N—N linked diimines (C=N–N=C). Azines are receiving increasing attention because of their chemical, physical and biological properties.[1] Our group works on a special class of azines which is 1,1-diaminoazines. This azine is synthesized by condensation reaction of aromatic aldehydes and aminoguanidine hydrochloride in water. Initially, this class of molecules was termed as guanylhydrazones; however, no attention was paid towards the azine tautomeric form. Our group performed quantum chemical and experimental studies to support the existence of azine tautomeric form which were wrongly present in other tautomeric form (hydrazone).[2] The presence of electrophilic and nucleophilic sites in the same molecule make 1,1-diaminoazines a unique substrate (I) for cycloaddition reactions synthesize dihydropyrazoles and different types of substituted triazoles.[3] 1,1-diaminoazines carry multifunctional characteristics these are due to (a) the conjugated double bonds, (b) the many active hydrogen atoms, (c) the N2 centre in 1,1-diaminoazines acts as a proton acceptor, and (d) the iminic C4 can act as a hydrogen bond donor.[4] Taken together, these features make 1,1-diaminoazines as bifunctional organocatalysts and thus can be employed in the catalysis of C-P and C-C bond formation.[5] The developed methodolgy is cheap and economic, these reactions can be carried out in aqueous medium. 1,1 Diaminoazines have been utilized in aldol/cascade cyclisation reactions and different MCRs. DFT studies supported the bifunctional organocatalytic characteristics of 1,1-diaminoazines. 4-pyridyl-4 methyl-1,1-diaminoazine was employed to generate the pincer complex with $Pd(OAc)_2$.The application of the complex in catalysing the medicinally important scaffold (e.g., Benzimidazoles, Quinolines) synthesis using the ADC mechanism has been reported.[6]

Fig.1. C-P bond formation using 1,1-diaminobenzalazine as an organocatalyst

Acknowledgement: This work was supported by grant No. BT/PR/40164 from the Dept. of Biotechnology (DBT), Government of India to PVB, for the computational part. The authors also thank the Centre of Excellence (COE-ABAV) at NIPER S.A.S. Nagar, supported by the Dept. of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Government of India.

[1]*Org. Biomol. Chem.* **2019**, *17*, 8486-8521.
[2]*J. Org. Chem.* **2016**, *81*, 7574-7583.
[3]*J. Org. Chem.* **2021**, *86*, 7659-7671.
[4]*Chem. Comm.* **2021**, *57*, 11717-11720.
[5]*Tetrahedron Lett.* **2023**, *122*, 15450.
[6]*Org. Biomol. Chem.* **2025**, *23*, 343-351.

CCS - D1 - O05

Hydrogen evolution suppression as a prerequisite for selective CO_2 reduction on MXene-supported single-atom catalysts

Sergio Posada-Pérez[1*], Gibu George[2], Sergio Moles-Quintero[1], Anna Vidal-López[2], Albert Poater[2], Miquel Solà[2], Mercedes Alonso[1], and Frank de Proft[1]

[1]*Algemene Chemie (ALGC), Vrije Universiteit Brussel (VUB), Belgium;* [2]*Institut de Química Computacional i Catàlisi, Universitat de Girona, Spain*

Two-dimensional materials such as MXenes and graphitic carbon nitride have emerged as versatile supports for atomically dispersed catalysts, offering strong metal–support interactions and well-defined coordination environments. These features enable the stabilization of isolated metal centers, making them attractive platforms for electrocatalytic reactions relevant to energy conversion.

However, reactions such as CO_2 reduction are inherently complex and inevitably compete with the hydrogen evolution reaction (HER), which often dominates the electrochemical response. Despite this, the computational prediction of electrocatalysts' performance is frequently discussed in terms of the overpotential required for CO_2 reduction. However, without controlled selectivity, the predictions offer limited practical relevance. In this context, understanding and suppressing HER is a necessary first step before assessing the true potential of a catalyst for CO_2 reduction.

Here, we systematically analyze HER on atomically dispersed metal sites supported on MXenes, with particular emphasis on $Ti_3C_2O_2$. A total of twelve different single-metal species were examined under varying surface chemistries, including different oxygen coverages and Ti vacancy concentrations. Our results show that the local environment of surface Ti vacancies plays a decisive role in governing HER activity. While most metal centers remain intrinsically or moderately active for HER across all surface conditions, Ru atoms anchored at high concentrations of Ti vacancy clusters markedly weaken hydrogen binding, leading to a pronounced suppression of HER.[1]

By explicitly placing HER at the center of the analysis, this work demonstrates that catalyst assessment must go beyond activity metrics alone. Only through a careful evaluation of competing reactions and selectivity constraints can atomically dispersed catalysts be meaningfully identified as viable candidates for selective CO_2 electroreduction.

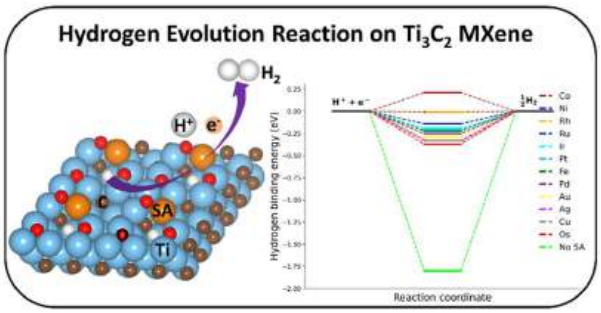

Fig. 1. Representation of SAC anchored on Ti_3C_2 MXene with O-termination and the reaction patway of HER, showing values close to 0.00 eV of proton binding energy when SAC is supported.

[1]George, G.; Moles-Quintero, S.; Poater, A.; Solà, M.; Alonso, M.; de Proft, F.; Posada-Pérez, S.; *Submitted*.

CCS - D1 - O06
Producing ethylene with light

Anna Fortunato and Francesca Arcudi
Dept. of Chemical Science, University of Padova, Italy

Ethylene, a key intermediate in ~60% of all plastics, is industrially produced via acetylene semi-hydrogenation. Conventional thermocatalytic routes dominate current industrial practice, despite limited selectivity and high operating temperatures, external H_2 feeds, and noble-metal (Pd-based) catalysts, limiting energy efficiency, safety, and sustainability.
This talk outlines three heterogenous photocatalytic platforms for the sustainable visible-light-driven semi-hydrogenation of acetylene to ethylene, illustrating how isolated single-metal sites enable precise control over activity and selectivity maximizing atom efficiency through *i*) a metal-organic framework incorporating a cobaloxime linker (ZrCo-MOF), *ii*) cobalt single-atoms on carbon nitride (Co-CN) or *iii*) a pyrene-based hydrogen bonded organic framework with embedded Cu atoms (Cu@HOF).
The ZrCo-MOF catalyst operates in tandem with a ruthenium-based photosensitizer, achieving quantitative conversion of acetylene to ethylene under an ethylene-rich gas stream, with high selectivity (>99.9%). Moving toward integrated platforms, two all-in-one photocatalytic systems are introduced. Combining light absorption and catalytic activity within a single material, eliminates the need for an external sensitizer. In the Co-CN system, cobalt single atoms anchored on carbon nitride act as isolated catalytic sites within a photoactive support affording continuous operation for over 40 days while maintaining >99.9% selectivity. Similarly, the Cu@HOF material integrates copper active sites within a water-stable hydrogen-bonded organic framework, allowing the rapid and highly selective removal of acetylene impurities within 75 minutes irradiation under ethylene-rich feeds, together with straightforward catalyst recovery and reuse.
Overall, these results highlight the potential of noble-metal-free, light-driven catalysts operating under mild conditions for this relevant chemical transformation, exemplifying crucial advancements in sustainable catalysis and offering distinct advantages over current hydrogenation technologies.

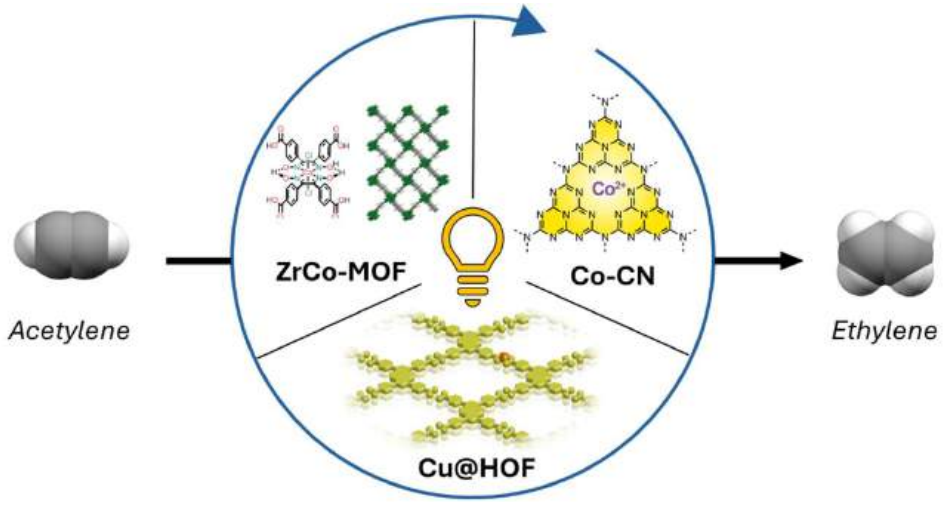

Fig. 1. Visible light powered semi-hydrogenation of acetylene to ethylene using (*i*) ZrCo-MOF, (*ii*) Co-CN, or (*iii*) Cu@HOF heterogeneous catalyst.

[1]A. Fortunato‡, A. E. B. S. Stone‡ (‡ equal contribution), X. Wang, E. Saggioro, R. Q. Snurr, J. T. Hupp, F. Arcudi and L. Đorđević, *Adv. Mater*. **2025**, *37*, 2408658.
[2]A. Fortunato, D. Perilli, A. Dron, V. Celorrio, G. Dražić, L. Đorđević, L. Calvillo, C. Di Valentin and F. Arcudi, *Small Methods*, **2025**, 2500527.
[3]A. Fortunato‡, B. Adranno‡ (‡ equal contribution), S. Silloni, M. Barbieri, S. Agnoli, L. Đorđević and F. Arcudi, *submitted*.

CCS - D1 - O07

Insights into 4-nitrostyrene chemoselective hydrogenation on Pd supported on $(TiW)_2AlC$ and $(TiW)_3AlC_2$ MAX phases and their corresponding MXenes

Mihaela-Mirela Trandafir[1], Bar Favelukis[2], Maxim Sokol[2], Mihaela Florea[1]
[1]National Institute of Materials Physics, Romania; [2]Tel Aviv University, Israel

Chemoselective hydrogenation of multifunctional molecules remains a key challenge in heterogeneous catalysis, where highly active metals such as palladium[1] often suffer from limited selectivity[2] and poor catalyst stability. Here, we demonstrate that Ti-W-based MAX phases and their corresponding MXenes act as distinct catalyst supports that fundamentally influence Pd selectivity and durability during the hydrogenation of 4-nitrostyrene. Palladium nanoparticles (0.5 wt.%) supported on $(TiW)_2AlC$ MAX phase and its derived $(TiW)_2CT_x$ MXene achieve complete conversion within 10 min with quantitative selectivity toward 4-ethylnitrobenzene and a turnover frequency of 3600 h^{-1}. In contrast, Pd supported on $(TiW)_3AlC_2$ and $(TiW)_3C_2T_x$ exhibits lower initial activity. Notably, while MAX-phase-supported catalysts undergo rapid deactivation upon recycling, the MXene-supported systems retain high activity and selectivity over at least four consecutive reaction cycles. This enhanced stability is attributed to stronger metal–support interactions in MXenes, promoted by their surface terminations (–O, –OH, –F) and higher surface polarity, which effectively anchor Pd nanoparticles. These findings highlight MXenes as superior supports for chemoselective hydrogenation, combining high activity with markedly improved catalyst durability, and provide insight into the role of surface chemistry in governing metal–support interactions.

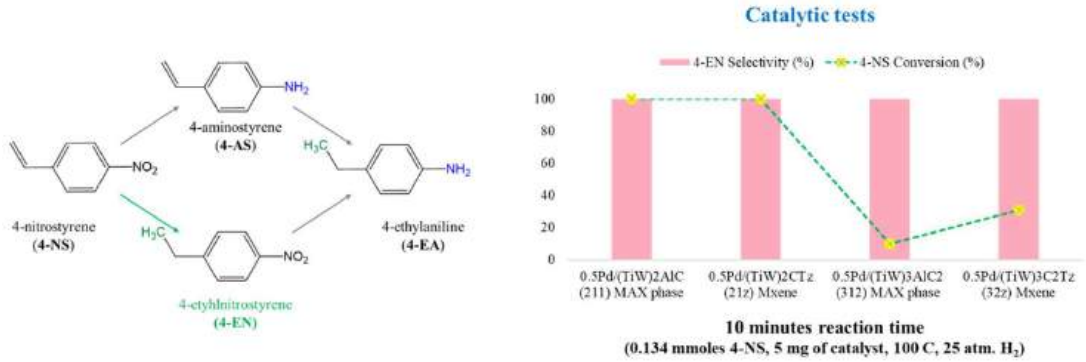

Fig. 2. Catalytic performance of MAX phase and MXene-based catalysts in 4-NS hydrogenation

This work was supported by the Romanian Ministry of Education and Research through the Core Program 2023-2026 (contract PC3-PN23080303); MMT and MF acknowledge the CNCS/CCDI-UEFISCDI for the PN-IV-P7-7.1-PED-2024-2346 project, within PNCDI IV.

[1]Trandafir, M.M.; Neaţu, F.; Chirica, I.M.; Neaţu, S.; Kuncser, A.C.; Cucolea, E.I.; Natu, V.; Barsoum, M.W.; Florea, M. *ACS Catal.* **2020**, *10*, 5899-5908.
[2]Serna, P.; Corma, A. *ACS Catal* **2015**, *5,* 7114-7121.

CCS - D1 - O08
Partial hydrogenation of alkynes using carbohydrates as alternative hydrogen source on Pt/C

Till De Cahsan[1], Claudia Schneider[1], Eszter Baráth[1]
[1]*Leibniz Institute for Catalysis e. V., Germany*

The selective semi-hydrogenation of alkynes is one of the most important organic transformations with wide applications.[1] The direct application of biomass in transfer hydrogenation reactions is beneficial because of renewability. Biomass derived hydrocarbons, such as sugars, cellulose, and starch, are potentially important feedstocks obtained by photosynthesis in plants from CO_2. For instance, glucose is inexpensive, easily obtained from natural renewable resources, and safe to handle. This method has the advantage of eliminating the use of pressurized H_2 gas and related pressure-accommodating experimental setups.[2]
The transfer hydrogenation of alkynes with carbohydrates exhibited a highly selective saturation pattern, where the cis-alkene was the predominant intermediate and the trans-alkene a minor product (Figure 1). The formation of the corresponding fully saturated product was not observed.
We analyzed the carbohydrate after the reaction. In a model reaction, we detected small, oxidized fragments like lactic acid, still intact six membered sugar molecules and oxidized six membered sugar rings.
We tested various carbohydrates for the transfer hydrogenation of internal alkynes in a wide substrate scope.
In order to determine the physical chemical parameters of the given reaction, diphenylacetylene, as model compound was studied. Kinetic analysis revealed initial reaction rates and activation parameters, including activation energy (E_a), activation enthalpy ($\Delta H^{\ddagger}$), and activation entropy ($\Delta S^{\ddagger}$).
Monosaccharides, disaccharides and polysaccharides were used successfully as H-donors in this model reaction.
Under optimized conditions 35 differently substituted internal alkynes were studied, the corresponding cis/trans alkenes were detected with good to excellent yields.
In order to utilize the sugar residue remaining after the reaction, we followed a protocol for the synthesis of bio-derived carbon with a high surface area, which can be used as a supporting material in catalyst synthesis.

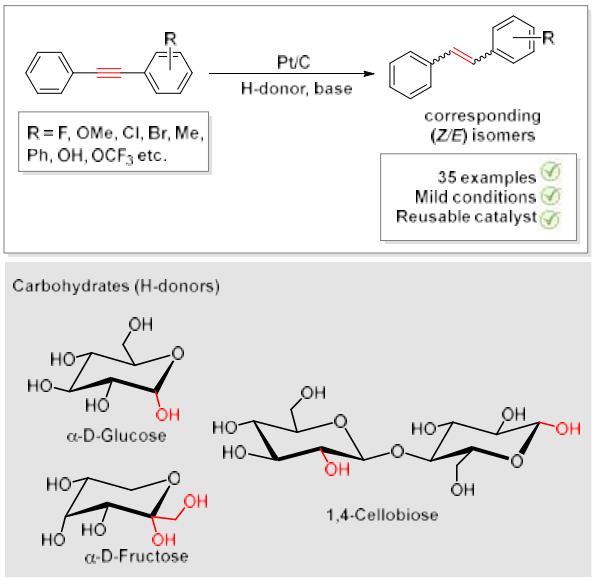

Fig. 1. Direct utilization of sugars to selectively reduce alkynes.

[1]Kusy R.; Grela, K. *Chem. Rev.* **2025**, *125* (9), 4397-4527.
[2]Manna S.; Antonchick A. P. *ChemSusChem* **2019**, *13*, 3094-3098.

CCS - D1 - O09

Catalytic hydrogenation and dehydrogenation reactions using molybdenum sulfide clusters and their sulfur-centered reaction mechanisms

Rosa Llusar*, Eva Guillamón, María Gutiérrez-Blanco, Juanjo Mateu-Campos, Mónica Oliva, V. Sixte Safont
Dept. de Química Física i Analítica, Universitat Jaume I, Spain

Incomplete cubane-type Mo_3S_4 clusters share structural features with the MoS_2 basal planes and can serve as molecular models of the active sites of this heterogeneous catalyst. Our group has shown that these Mo_3S_4 complexes are efficient catalysts for the direct hydrogenation and silane transfer hydrogenation of nitro- and azoarenes to produce anilines. In this presentation, the catalytic performance of these complexes for the (*Z*)-selective semihydrogenation of internal alkynes, hydrogenation of sulfoxides to sulfides and methanolysis of silanes will be analyzed.[1-3] Our results support the operation of a sulfur-centered reaction mechanism for the hydrogen H-H and hydrosilane H-Si bond activation to afford a bis(hydrosulfide) intermediate, as shown in Figure 1. Once the $Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2$ intermediate is formed, hydrogen is transferred to the organic substrate, alkyne or sulfoxide, or released in the case of the methanolysis of hydrosilanes. Special emphasis will be given to the reaction mechanisms of these transformations. All our mechanistic proposals are framed as cluster catalysis and based on a combined experimental and theoretical approach.

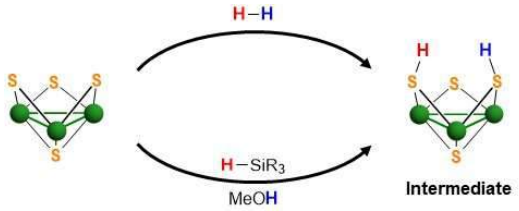

Fig. 1. Formation of the bis(hydrosulfide) intermediate

The financial support from the Spanish Ministerio de Ciencia e Innovación (PID2022-141089NB-I00) and Generalitat Valenciana (CIAICO/2024/94) is greatfully acknowledged.

[1]Gutiérrez-Blanco, M; Algarra, A. G.; Guillamón, E.; Fernández-Trujillo, M. J.; Oliva, M.; Basallote, M. G.; Llusar; R.; Safont, V. S. Inorg. Chem. **2024,** 63, 1000-1009..
[2]Mateu-Campos, J; Gutiérrez-Blanco, M.; Guillamón, E.; Safont, V. S.; and R. Llusar, Catal. Sci. Technol., 2024, 14, 6845-6853.
[3]J. Mateu-Campos, M. Gutiérrez-Blanco, E. Guillamón, V. S. Safont, J. Benet-Buchholz and R. Llusar Inorg. Chem. 2025**,** ***64,*** 6552-6560.

CCS - D1 - O10

Photoredox defluorinative γ-substitution: Trading C–F for C–C bonds towards monofluoroalkenes

Jean-Denys Hamel[1,2]

[1]University of Lethbridge, Canada; [2]Canadian Centre for Research in Advanced Fluorine Technologies, Canada

As the C–F bond is the strongest single bond carbon makes with any element, its selective cleavage in the presence of an abundance of much weaker bonds is a challenge, and one that we must tackle rapidly to better utilize and dispose of organofluorine compounds. Reactions that leverage partial defluorination are particularly attractive to attain fluorinated motifs that are otherwise challenging to synthesize. Of particular interest to our group are monofluoroalkenes, which can be used in pharmaceutical development as non-hydrolyzable isosteres of amides and enols of fixed configuration. In this context, we investigated photoredox transformations involving allylic C–F bond functionalization as a strategy to prepare monofluoroalkenes for allylic difluorides. We revealed that a broad range of radical precursors are amenable to such defluorinative C–C bond formation, and that the system retains high performance whether metal-based or organic photocatalysts are used.

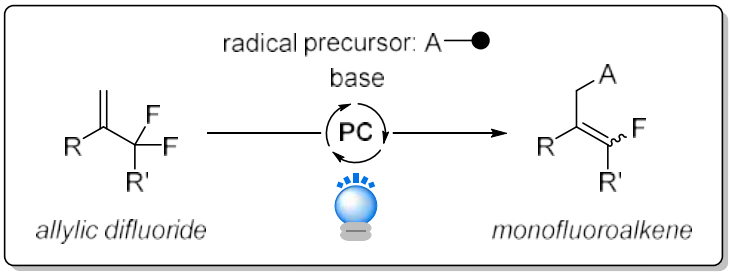

Fig. 1. Photoredox γ-substitution of allylic difluorides

CCS - D1 - O11

Visualizing the surface restructuring of copper electrodes during CO_2 electro-reduction

Hui Wang[1], Ward van der Stam[1], Laurens D.B. Mandemaker[1], Christos Chatzilias[1], Jiaorong Yan[1], Thomas Hartman[1], Bert M. Weckhuysen[1,*]

[1]Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry, Dept. of Chemistry, Faculty of Science, Utrecht University, The Netherlands

Dynamic surface restructuring of copper electrodes under electrochemical CO_2 reduction reaction conditions results in continuously modified active sites, profoundly affecting both catalyst stability and selectivity.[1,2] To design the optimal electrocatalyst material, real-time monitoring of the generation of active surfaces, their structure under prolonged operational conditions, and their regeneration becomes crucial. In this work, we reveal the dynamic surface restructuring at moderate cathodic bias, and the self-healing ability of copper electrodes at low cathodic bias, by employing in-situ and operando electrochemical atomic force microscopy (**Figure 1a**). We find that copper dissolution occurs at the electrode-electrolyte interface due to strong interactions with the reaction intermediates, resulting in a liquid-like region close to the surface. However, the dissolved copper species rapidly redeposit at low cathodic bias during potential modulation experiments (**Figure 1b**). We propose a dynamic and potential-dependent equilibrium between Cu dissolution and redeposition, forming a liquid-phase region near the interface, which gives rise to the self-healing ability for the Cu electrodes (**Figure 1c**). The self-healing ability can be broken in two ways: (1) the presence of organic ligands that capture dissolved copper and transport it away from the electrode surface, and (2) high concentrations of products (e.g., formate). We propose the existence of a liquid-phase region very close to the active electrode surface, where dynamic copper dissolution-redeposition occurs, that needs to be maintained through dynamic operation (e.g., pulsed electrolysis) for stable operation. Our findings present a paradigm shift: to circumvent copper degradation, we do not need to design stable materials, but rather stable operational conditions.

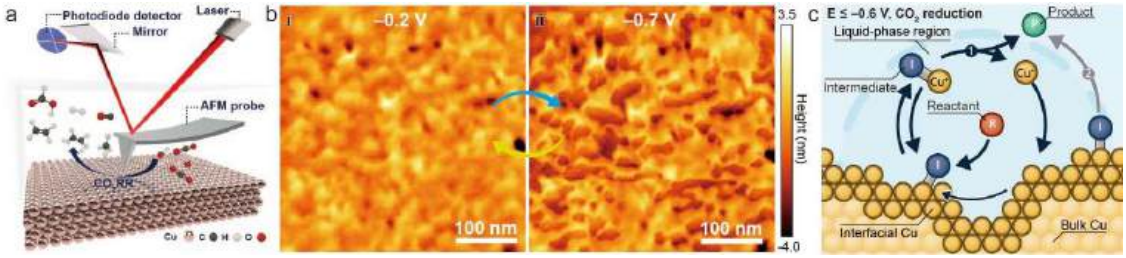

Fig. 1. (**a**) Schematic diagram of in-situ electrochemical atomic force microscopy (EC-AFM) for revealing the surface restructuring during electrochemical CO_2 reduction reaction. (**b**) In-situ EC AFM images of Cu electrode in the CO_2-saturated 0.1 M $KHCO_3$ under (i) –0.2 V and (ii) –0.7 V vs. RHE. (**c**) Schematic diagrams presenting the dissolution-redeposition equilibrium in the liquid-like region near the Cu-electrolyte interface, which contributes to the self-healing restructuring of Cu electrode.

[1]J. Kok, P. P. Albertini, J. Leemans, R. Buonsanti, and T. Burdyny, *Nat. Rev. Mater.* **2025**, 10, 550-563.

[2]H. Wang, L. D. B. Mandemaker, J. de Ruiter, X. Yu, W. van der Stam, and B. M. Weckhuysen, *Angew. Chem. Int. Ed.* **2025**, 64, e202424530.

CCS - D1 - O12

Sustainable chemical recycling of polycarbonate: Solvent-assisted methanolysis using magnetic Fe@ZIF-8 derivatives

Shun-Han, Chuang[1], Yu-Tzu Chang[1], Ren-Xuan, Yang[1*]
[1]*Institute of Environmental Engineering and Management, National Taipei University of Technology, Taiwan*

As global polycarbonate (PC) consumption continues to rise, developing efficient and sustainable chemical recycling strategies to recover virgin-like monomers is crucial for achieving circular polymer economies and reducing plastic waste. Herein, a magnetic and reusable potassium carbonate-modified iron-loaded on a zeolite imidazolate framework (ZIF) catalyst (K_2CO_3/Fe@ZIF-8) was synthesized for low-temperature PC methanolysis under atmospheric pressure. The introduction of tetrahydrofuran (THF) as a co-solvent was also studied, which can enhance PC solubility and accelerate methanol diffusion. By the reaction over 0.15 g of 30 wt.%K_2CO_3/Fe@ZIF-8 catalyst, 100% PC conversion and 99% bisphenol A (BPA) yield were achieved within 30 min at 60 °C. The catalyst possessed an apparent activation energy (E_a) of 51.38 kJ mol^{-1}, which is the lowest reported value for heterogeneous catalysts to date. Furthermore, K_2CO_3/Fe@ZIF-8 catalysts can be easily recovered and reused through simple magnetic separation. The reusability test demonstrated that the catalyst maintained high activity and selectivity over five cycles, preserving 94.06% PC conversion and 89.27% BPA yield. This study provides a low-energy, magnetically separable catalytic platform enabling scalable and sustainable PC depolymerization under mild and environmentally benign conditions.

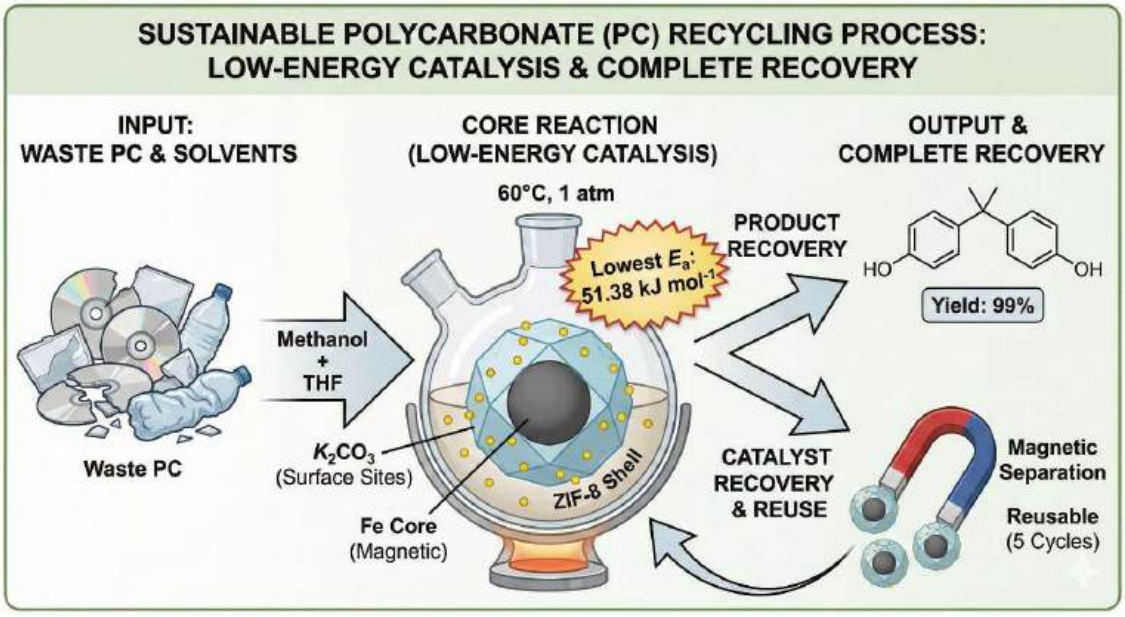

Fig. 1. Schematic illustration of Sustainable Chemical Recycling of Polycarbonate: Solvent-Assisted Methanolysis using Magnetic Fe@ZIF-8 Derivatives

CCS - D1 - O13
Heterogeneous reductive hydroformylation via amine/Rh-based solid molecular catalysts

Keanu V.A. Birkelbach[1,2], Jeroen T. Vossen[3], Andreas J. Vorholt[3], Regina Palkovits[1,2,3]
[1]Institute for a Sustainable Hydrogen Economy, FZJ GmbH, Germany; [2]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Germany; [3]Max Planck Institute for Chemical Energy Conversion, Germany

Solid molecular catalysts (SMCs) are heterogeneous materials featuring molecularly defined active sites. They are commonly received by immobilizing a metal precursor *via* a polymer containing appropriate ligand motifs, so-called macroligands. SMCs thus aim to combine the process-related advantages of heterogeneous catalysts with the improved reactivity of homogeneous ones.[1,2]
The reductive hydroformylation is an important industrial process to produce alcohols from olefins. Since the hydroformylation is a homogeneously catalyzed reaction, down-stream processing and catalyst recycling often come at significant energy cost and complexity.[3]

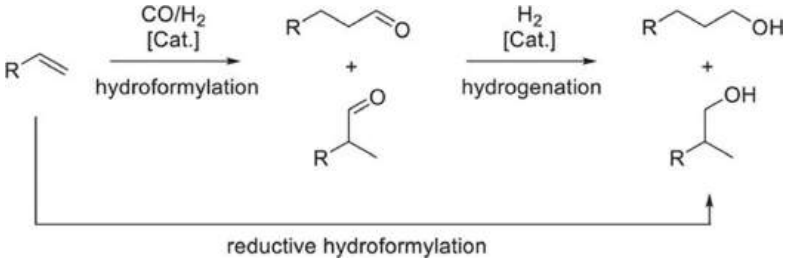

Fig. 1. Stepwise and concerted reaction from olefins towards alcohols.

We present SMCs based on amine-containing macroligands and rhodium precursors which offer a heterogeneous alternative.[4] Through an iterative macroligand design process, hydrogenation activity is first unlocked and subsequently significantly improved, yielding a best-performing SMC which converts 1-octene to >99% alcohols in a solvent-free environment without any hydrogenation of the starting aldehyde. Using optimized reaction conditions, the SMC was successfully recycled over 12 consecutive runs, maintaining activity and exhibiting perpetual metal loss as low as 1.2%. An upscaled, time-resolved experiment was used to investigate the correlation between conversion and *n:iso*-ratio, also confirming an auto-tandem catalytic mechanism. The composition and nature of the active site was investigated using a combination of SS-MAS-NMR, XPS, DRIFTS and high-resolution imaging. Besides the expected Rh-carbonyl complexes, findings suggest the formation of multinuclear, neutral or anionic species, the formation of which was previously reported for the homogeneous analogue.

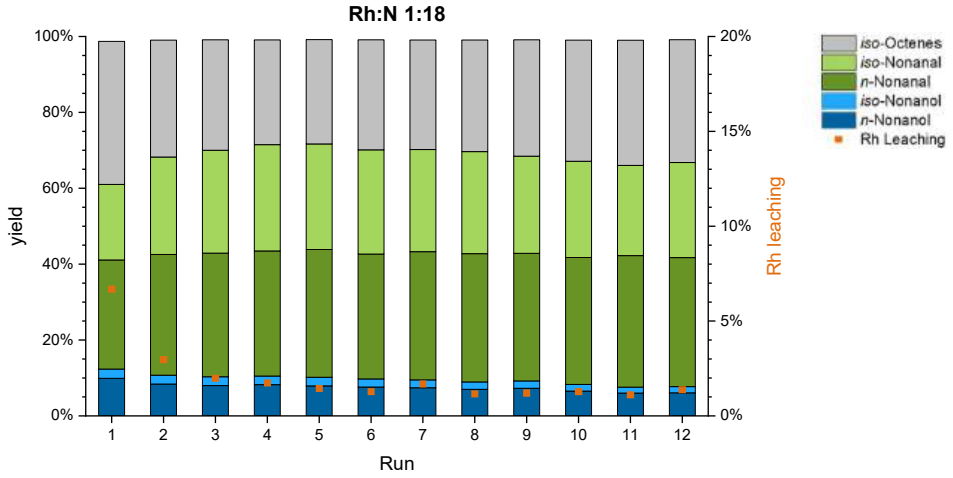

Figure 2 Yields and Rh leaching in recycling experiments encompassing 12 runs. *In situ* catalyst formation with **APIII** (247 g mol_N^{-1}) and [Rh(acac)$(CO)_2$] (0.1 mol% referred to the substrate) at a pressure of 75 bar ($CO:H_2$ = 25:50) and 700 rpm stirring speed for 4 h in 20 mL autoclave reactors. Analyzed by GC-FID and XRF.

Acknowledgements: We thank Werner Siemens Foundation for funding in the frame of the WSS research center catalaix – catalysis for a circular economy. This work was also supported by the Cluster of Excellence Fuel Science Center (EXC 2186, ID: 390919832) funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities. The authors acknowledge the funding by the German Federal Ministry of Research, Technology and Space (BMFTR) and the Ministry of Economic Affairs, Industry, Climate Action and Energy of the State of North Rhine-Westphalia through the project HC-H2.

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CCS - D1 - O14

3D micro-extrusion of structured oxide catalysts: Linking catalyst shaping to reactor-relevant performance

Yoran De Vos[1], Jurjen Cazemier[1], Arturo Pajares[1], Luca Mastroianni[1], Marta Sagredo-Acitores[2], Susana Perez-Gil[2], Vesna Middelkoop[1], Linsey Garcia-Gonzalez[1]

[1]Flemish Institute for Technological Research – VITO NV, Belgium; [2]TECNALIA R&I, Spain

Heterogeneous catalysts come in many shapes and sizes. Typical shapes such as pellets or extrudates often impose trade-offs between pressure drop, heat management, and catalyst effectiveness factors. These limitations are particularly evident for highly exothermic reactions, such as Fischer-Tropsch synthesis and CO_2-methanation, where transport effects and temperature gradients can strongly influence performance. Additive manufacturing provides new opportunities to explore catalyst shapes and architectures beyond those accessible by conventional shaping.

In this work, we demonstrate the use of 3D micro-extrusion to shape structured catalysts with tailored architecture, porosity and textural properties, while maintaining compatibility with established catalyst materials. By tuning these design variables (architecture, porosity, textural properties) relatively low pressure drop structures can be combined with good mass transport enabling effective use of the active catalyst material. Importantly, the technology is shown to be compatible with scaling to reactor-relevant dimensions.

The potential of this methodology is illustrated using two representative case studies. In a first example, TiO_2-supported CO_2-methanation catalysts with tuneable porosity were fabricated and their structure-performance relationship was evaluated without changing their chemical composition. In a second example, conducted within the HEU CARBIOW project, 3D-micro-extrusion was applied to the development of 3D-printed Co-Ru Al_2O_3-supported Fischer-Tropsch catalysts (Fig.1a) designed for a TRL5 millichannel reactor, which made it possible to produce advanced aviation biofuels (Fig.1b).

Together, these examples highlight how 3D micro-extrusion printing enables systematic exploration of catalyst architecture at scales relevant for reactor studies. This approach provides a flexible platform to bridge catalyst formulation, shaping, and reactor performance, offering new opportunities for the development of structured catalysts for demanding catalytic processes.

This work is part of the CARBIOW project, which is supported by Horizon Europe under grant agreement 101084443.

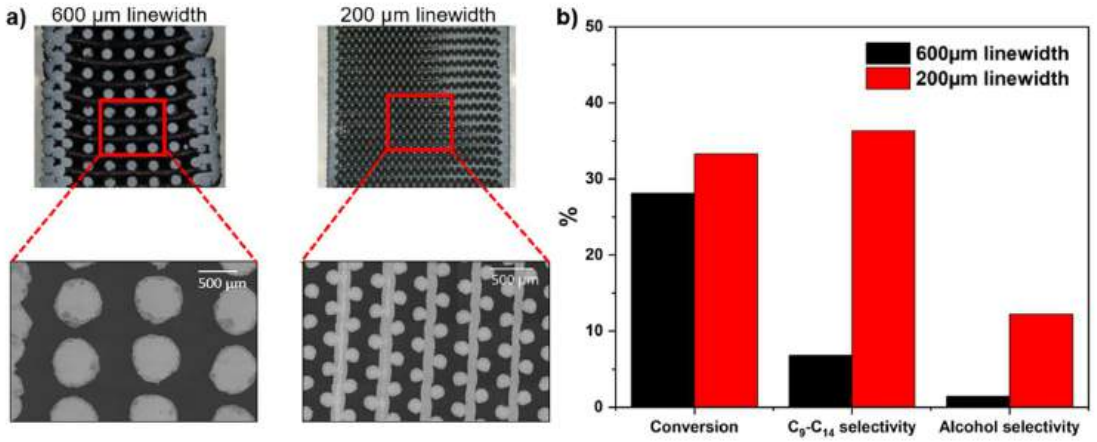


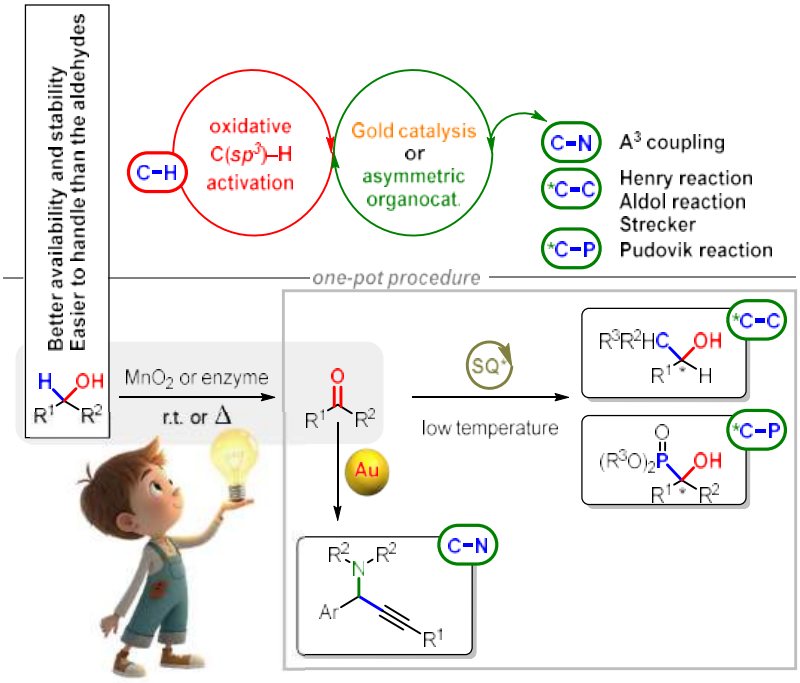
Figure 1. (a) SEM cross sections of embedded Fischer-Tropsch catalysts with 600 µm and 200 µm printed fiber linewidths, (b) CO conversion and carbon-based selectivities towards advanced biofuels under identical reaction conditions (250°C, 20 bar, H_2/CO=2). Data were obtained at comparable conversions using adjusted space velocities.

CCS - D1 - O15

Innovations in enantioselective organocatalytic C–P and C–C bond formation using formal C(sp³)–H activation

Sandra Ardevines[1], Juan V. Alegre-Requena[1], Christian Ascaso-Alegre[1], Stefania Perulli[2], M. Concepción Gimeno[1], Juan Mangas-Sánchez[3], Olga García Mancheño[2], Eugenia Marqués-López[1], Raquel P. Herrera[1]
[1]Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC-University of Zaragoza, Spain; [2]Organic Chemistry Institute, University of Münster, Germany; [3]School of Chemistry, University of Oviedo, Spain

Many organic reactions involving aldehydes lead to products of biological interest. However, aldehydes are easily contaminated over time by traces of their corresponding carboxylic acids, which can inactivate organocatalysts, as observed during our previous Henry protocol development.[1] Motivated by this observation, we explored the possibility of producing aldehydes *in situ* by oxidizing the corresponding alcohols.[2] Alcohols are more convenient than aldehydes, mainly due to their higher availability, stability, and ease of handling. The transformation of alcohols into the corresponding carbonyl compounds for subsequent reaction with nucleophiles in an organocatalytic and enantioselective manner has been scarcely investigated.
Herein, we present the pioneering work and the first organocatalytic enantioselective aldol,[2] Henry,[2,3] Pudovik,[3,4] or Strecker[5] reactions starting from alcohols through a formal C(sp³)-H activation, all of them important methods for forming C-C and C-P bonds in organic synthesis.



We would like to thank the Agencia Estatal de Investigación (AEI), for the financial support of projects PID2020-113351RA, PID2020-117455GB-I00, PID2022-136861NB−I00 and PID2023-147471NB-I00 funded by MICIU/AEI/10.13039/501100011033, and Gobierno de Aragón-Fondo Social Europeo (Research Group E07_23R). The Deutsche Forschungsgemeinschaft (DFG, project GA1594/6-2) is acknowledged for generous support.

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CCS - D1 - O16
One-electron approach for trans-selective alkyne semi-reduction via cobalt catalysis

Samer Gnaim
Weizmann Institution of Science, Israel

Selective partial reduction of alkynes to alkenes is a cornerstone of synthesis, yet broadly applicable catalytic routes to E-configured products remain scarce. We report a cobaltcatalyzed electrochemical platform that converts internal alkynes to trans-alkenes with high stereoselectivity via a radical pathway. The method accommodates diverse electronic and steric environments, delivers excellent chemoselectivity and functional-group tolerance, and enables straightforward access to trans-deuterated products. It also operates selectively in substrates bearing multiple alkyne motifs. Mechanistic studies-cyclic voltammetry, UV-vis spectroelectrochemistry, and DFT-support a dual catalytic cycle in which cathodic generation of a Co-H species engages an organometallic radical relay to forge E-alkenes. Guided by these insights, we developed a complementary, purely chemical oxidative variant that provides E-alkenes from substrates unreactive under electroreductive conditions. Together, these results establish a general cobalt-based strategy for accessing stereodefined trans-alkenes and open a new avenue for radical-mediated alkyne functionalization.

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CCS - D1 - O17
Infrared Irradiation assisted Pd/Cu catalysis for sustainable C-N cross coupling

Ambra M. Fiore[1], A. Punzi[1], Pietro Cotugno[1], Gianluca M. Farinola[1]
[1]University of Bari "Aldo Moro", Italy

The increasing emphasis on green synthetic methodologies has driven the development of environmentally sustainable approaches for the synthesis of organic compounds. Among alternative energy sources, infrared (IR) irradiation has emerged as a powerful and efficient tool, offering clear advantages over conventional thermal heating.[1] When employed under solvent-free or environmentally benign conditions, IR irradiation enhances energy efficiency while minimizing reaction waste, in close accordance with the principles of green chemistry.[2,3,4]

Within this context, we report a practical and efficient Pd/Cu-catalyzed Buchwald–Hartwig amination assisted by IR irradiation under quasi-solvent-free conditions.[5] The reactions are performed in a non-anhydrous medium, open to air, using a stoichiometric amount of cyclopentyl methyl ether as solvent. This protocol enables high-yielding C–N cross-coupling reactions of aryl iodides and bromides with a broad range of secondary amines under mild conditions.

The cooperative Pd/Cu catalytic system allows for reduced palladium loading (as low as 1.5 mol%) and significantly shortened reaction times (1–3 h), while maintaining excellent functional group tolerance and broad substrate scope. Notably, this study represents one of the most relevant and environmentally friendly applications of IR irradiation in Pd/Cu co-catalyzed C–N cross-coupling reactions reported to date. Overall, the proposed methodology offers an economical, rapid, and broadly applicable route to aryl amines, providing a practical and sustainable alternative to traditional heating methods and contributing meaningfully to the advancement of green chemistry and environmentally responsible synthetic strategies.

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CCS - D1 - O18

Functionalized carbon and silica supports for C–H bond-activating enzymes immobilization and reuse

F. Careddu[1,2], C. Pontremoli[1], Kelsi R. Hall[3,4], M. Sørlie[3], V. G. H. Eijsink[3], C. Barolo[1], S. Bordiga[1]
[1]University of Torino, Torino, Italy; [2]University School for Advanced Studies IUSS Pavia, Italy; [3]Norwegian University of Life Sciences, Ås, Norway; [4]University of Canterbury, New Zealand

Lytic polysaccharide monooxygenases (LPMOs) are mononuclear copper-dependent enzymes that catalyze the oxidative cleavage of glycosidic linkages in polysaccharides, making them attractive catalysts for oxidative biotransformations. However, their industrial application is limited by pronounced sensitivity to oxidative inactivation, particularly under substrate-free conditions1,2.

Immobilization on solid supports represents an effective strategy to enhance LPMO stability, being a simple, economical that preserves enzymatic activity. Among the various supports explored for bio-conjugation, carbon nanotubes (CNTs) represent a promising option due to their commercial availability, low cost, and ease of surface targeted functionalization.

In this work, two engineered LPMOs - ScAA10C from Streptomyces coelicolor A3 and LsAA9A from Lentinus similis - were covalently immobilized onto carboxyl-functionalized MWCNTs via EDC/NHS chemistry, targeting surface-accessible lysine residues to promote confinement of the enzyme active site3. To investigate the effect of spatial confinement on catalytic behavior, different spacer molecules were employed. The immobilized enzymes retained oxidase, peroxidase, and peroxygenase activities and exhibited enhanced resistance to oxidative stress and thermal denaturation compared to the soluble enzymes.

However, the fine dispersion of CNT-based supports in solution hindered catalyst separation and reuse. To overcome this limitation, functionalized mesoporous silica nanoparticles were evaluated as alternative carriers due to their favorable separation properties and established biocompatibility. Immobilization on silica supports resulted in comparable activity retention while significantly facilitating catalyst recovery and recyclability for up to six oxidase cycles.

Overall, this study demonstrates that morphological and structural optimization of support materials is crucial not only for modulating LPMO activity and stability but also for enabling efficient catalyst recovery and reuse, thereby advancing durable and sustainable LPMO-based biocatalysts for industrial applications (e.g. waste valorization).

Acknowledgements: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme under the grant agreement n° 856446 (https://www.cube-synergy.eu). C.P., F.C., C.B., S.B. acknowledge support from the Project CH4.0 under the MUR program “Dipartimenti di Eccellenza 2023-2027” (CUP: D13C22003520001).

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CCS - D1 - O19

Iridium-free dual photoredox catalysis based on carbon nitride for greener C–C cross-couplings

Miguel M. de Vries Ibáñez[1], Gianvito Vilé[1]

[1]*Dept. of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Milano, Italy*

Visible light-driven dual photoredox catalysis, which combines photoabsorbers and transition-metal complexes, is a powerful tool for a broad range of cross-coupling reactions.[1] However, resource availability and industrial applicability of such processes remain challenging, due to the reliance on precious-metal containing light absorbers (e.g., Ir complexes) or homogeneous photocatalysts, which hamper downstream processing and increase production costs. Carbon nitride (CN_x), an heterogenous photocatalyst from abundant precursors like melamine or urea, has emerged as an alternative to homogeneous photocatalysts.[2] Moreover, its visible light activation offers the potential for integrating synthetic methodologies with solar energy. Despite the benefits, such novel materials have not been truly investigated within the organic synthetic space, leaving much room for exploration and discovery.[3]

In this study, we introduce the combination of CN_x and nickel complexes for cross-coupling reactions via both decarboxylation and C–H activation. Catalytic experiments under optimized conditions demonstrated the efficiency and selectivity of our system, showcasing the recyclability and robustness of the CN_x photocatalyst over five cycles. This method exhibited broad tolerance, achieving C(sp^3) functionalization in over 50 examples, including pharmaceuticals such as fenofibrate, caffeine and levodopa, with yields of up to 93%. The experimental findings are supported by Stern–Volmer experiments, electron paramagnetic resonance (EPR) analysis, and density functional theory (DFT) calculations, providing key structural and mechanistic insights into the catalytic system's behavior under visible-light irradiation. Our findings provide an understanding of the structure and performance of heterogeneous CN_x, paving the way for more sustainable, light-driven protocols for the synthesis of valuable compounds.

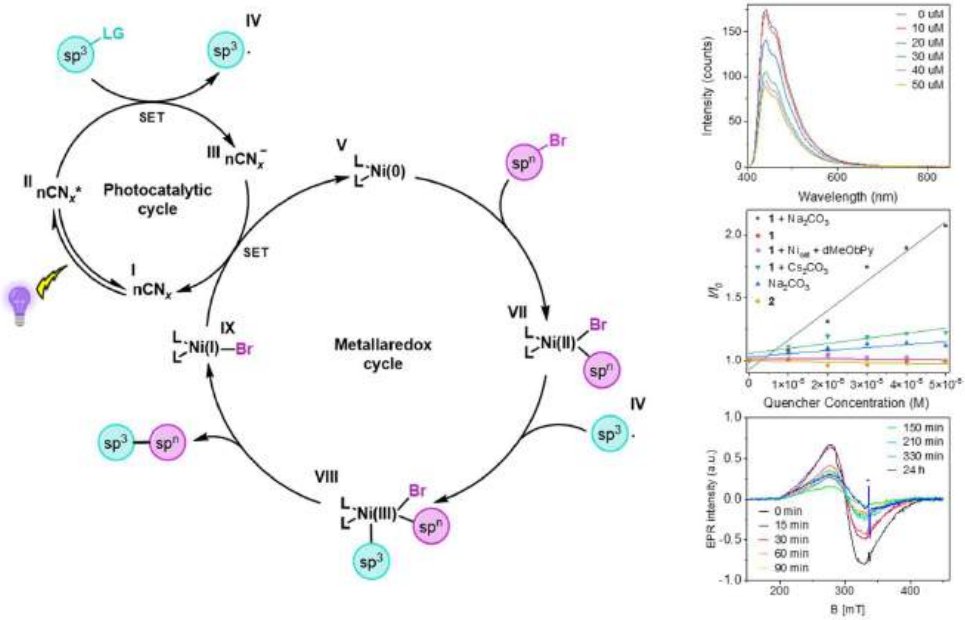

Fig. 1. Decarboxylative and C-H activation cross-coupling reactions general scheme using a homogeneous nickel complex and heterogeneous carbon nitride photocatalyst.

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CCS - D1 - O20
Single-atom functionalized poly(heptazine imide) as a platform for solar-to-chemical conversion

Luis FernandoGuimarães Noleto[1], Guilherme F.S.R. Rocha[1], Marcos Augusto Ribeiro da Silva[1], Izadora R. Menezes[1], Gabriel A. A. Diab[1], Ivo F. Teixeira[1]
[1]Dept. of Chemistry, Federal University of São Carlos, Brazil

The transition to a sustainable energy matrix faces significant challenges, such as grid instability due to the intermittency of renewable sources. While green hydrogen is pivotal for decarbonizing the chemical industry, direct solar-to-chemical conversion offers a compelling, albeit underestimated, alternative pathway to valorize abundant solar energy. This work demonstrate that Poly(heptazine imide) (PHI), a class of ionic, crystalline carbon nitride semiconductors, can bridge the gap between solar harvesting and chemical synthesis.[1, 2] By leveraging a cation exchange strategy, we show how metal Single-Atom Catalysts (SACs)—such as Fe, Ni, and Mn—can be stabilized within the PHI framework (**Figure 1**) to create precise active sites and tune band structures (**Figure 2a**).[3]

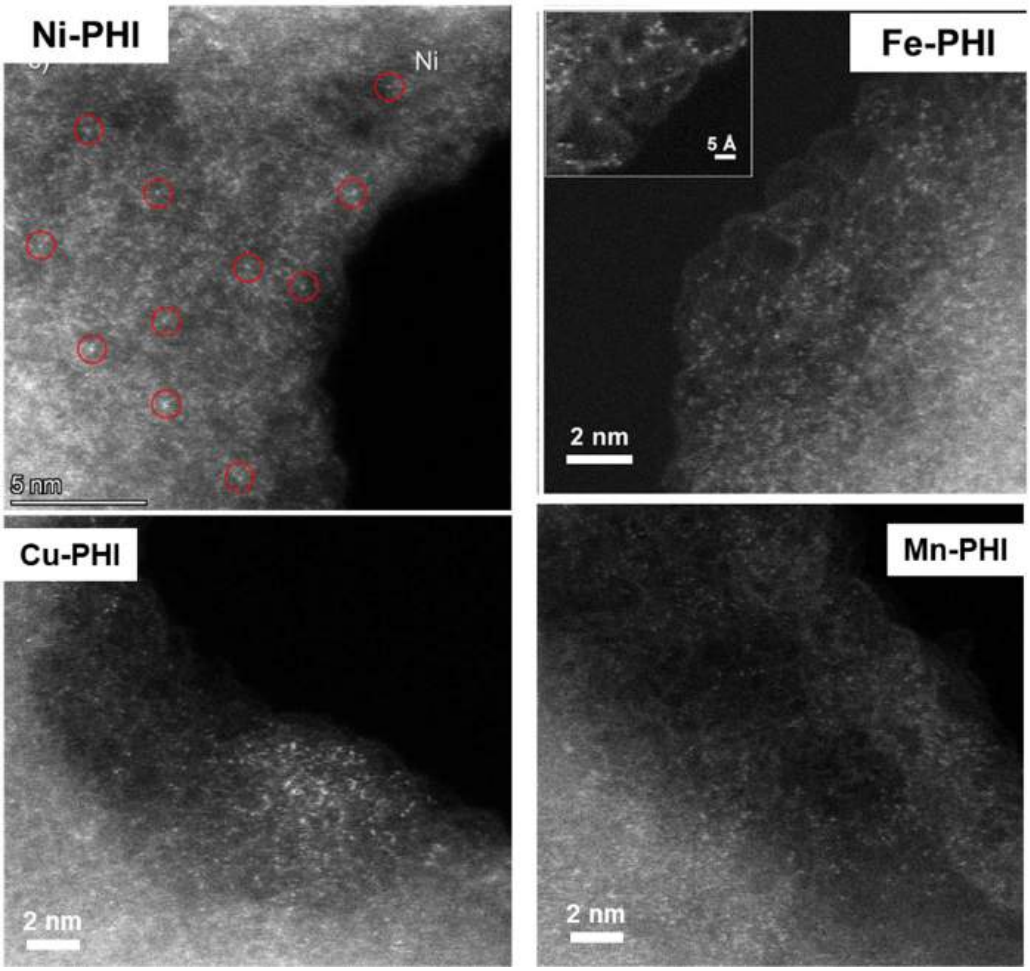

Fig. 1. STEM-HAADF images showing the stabilization of various metal Single-Atoms (Ni, Fe, Cu, Mn) within the poly(heptazine imide) (PHI) matrix.

Here, a series of recent examples developed by our research group are presented, demonstrating that these tailored photocatalysts can be successfully employed to drive the synthesis of commodity chemicals (**Figure 2b)**. For example, the production of Green Hydrogen, showing that Nickel-based PHI catalysts (Ni-PHI) can effectively replace costly platinum, challenging the economic feasibility barriers of conventional photocatalysis. Second, we illustrate the versatility of these materials in organic synthesis through the selective photoreduction of phenylacetylene to styrene under mild conditions.[4] Finally, we report on the sustainable production of hydrogen peroxide (H_2O_2) using H-PHI and Na-PHI, utilizing glycerol as a sacrificial reagent. These examples collectively demonstrate that single-atom functionalized carbon nitrides can drive a "solar-to-chemical" industry, offering a disruptive solution to safeguard the transition toward a low-carbon economy.

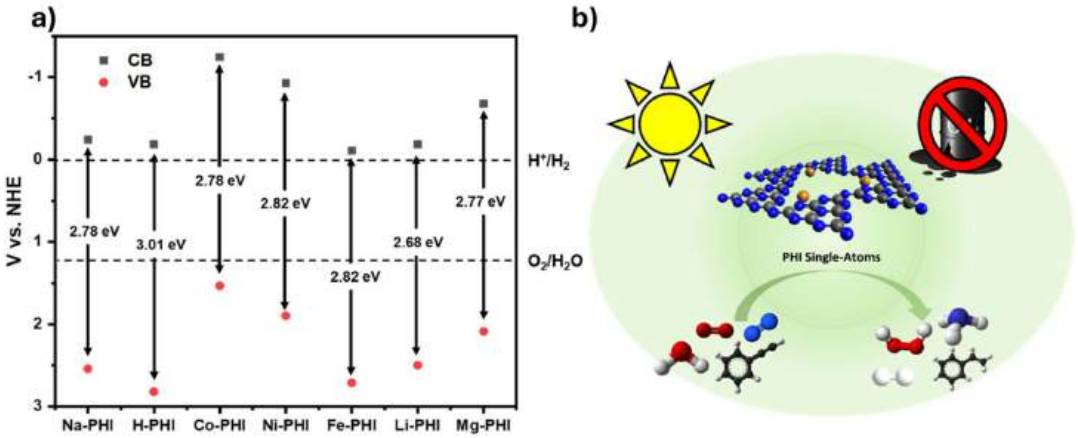

Fig. 2. (a) Band structure alignment and calculated potentials (vs. NHE) for different metal-functionalized PHI materials, demonstrating the tunability of Conduction and Valence Bands (CB/VB). **(b)** Schematic illustration of the PHI-based platform for solar-to-chemical conversion, highlighting applications in hydrogen evolution, organic synthesis (styrene production), and hydrogen peroxide synthesis.

Acknowledgements: This research was financially supported by the Brazilians funding agencies CAPES, CNPq (403064/2021 and 405752/2022), FAPESP (2020/14741-6, 2021/11162-8, 2024/00839-5 and 2021/12394-0) and FINEP (01.23.0645.00 and 01.23.0662.00). The authors are grateful to LNNano (EM-20210344 and TEM-C1-20232675).

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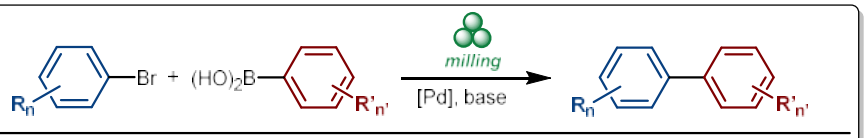
CCS - D1 - F01
Solvent-free mechanochemical Suzuki-Miyaura coupling

Ihar E. Mikhnavets[1], Yaxu Liu[1], Roman V. Larkovich[1], Catherine S. J. Cazin[1]
[1]*Ghent University, Belgium*

Organic solvents constitute a significant portion of chemical waste generated by synthesis. It reaches 85-90% of process mass contribution in the pharmaceutical sector. The pursuit of sustainability in chemical processes necessitates the reduction of solvent use and the adoption of environmentally benign synthetic protocols.[1] Mechanochemistry proved itself as a powerful synthetic tool to allow solvent-free transformations, however, significant amounts of solvent are used in product purification step, which undermines the "solvent-free" nature of the process.[2–5]
In order to exclude solvent use, we developed a solvent-free mechanochemical Suzuki-Miyaura cross-coupling protocol employing well-defined Pd-precatalysts which enable the efficient coupling of various aryl bromides with arylboronic acids at ultra-low catalyst loadings at room temperature. Sublimation was implemented as a solvent-free product isolation technique, which, in most cases, provides comparable or superior yields to traditional liquid chromatography. Assessment of environmental impact metrics (E-factor, DOZN score) of the process shows significant increase in sustainability for the sublimation-based workup, emphasising the environmental benefits of this approach.[6]
In addition, a head-to-head comparison of ball mill types (planetary *versus* mixer) delineates that reaction's outcome cannot be solely rationalized in terms of mechanical energy transfer.



Catalyst	Loading	Isolation and purification	E-factor	DOZN score
State-of-the-art	2-3 mol% Pd	Extraction + Chromatography	760-6255	57-59
Our catalyst	**0.05 mol% Pd**	**Sublimation**	**2-10**	**1-3**

Figure 1. Sustainable mechanochemical Suzuki-Miyaura reaction

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CCS - D1 - F02

An electrogenerated base route towards the synthesis of transition metal NHC-ligated complexes

Roman V. Larkovich[1], Ihar E. Mikhnavets[1], Henk Vrielinck[1], Catherine S.J. Cazin[1]
[1]*Ghent University, Belgium*

N-Hererocyclic carbenes (NHC) ligated metal complexes have dominated the field of transition metal catalysis to become widely used (pre-)catalysts in the pharmaceutical and fine chemical industry.[1] As a result, a lot of attention has been devoted to the development of versatile and sustainable methods for the synthesis of these complexes.

All common methods for the installation of NHC ligands onto corresponding metal precursors include the use of an external base that deprotonates the imidazolium salt.[2] Electrochemical strategies constitute elegant alternatives, eliminating the need for a base. However, the scope of the metals whose complexes are accessible via existing electrochemical methods is limited to those able to act as sacrificial anodes, with the released metal cations being the metal source.[3]

To address these limitations, we have developed novel methodologies that consist in electrogenerating bases from air, enabling carbene formation and its subsequent coordination. This strategy was found applicable to group 9-11 transition metals, without the need for a sacrificial anode as a metal source, and proved applicable to metals that are otherwise incompatible with direct electrolysis conditions.[4,5]

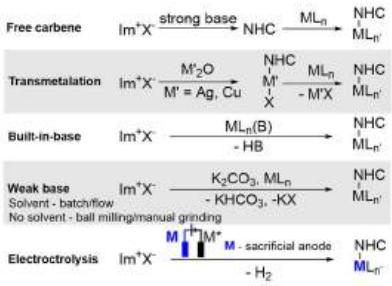

Figure 1. Most common synthetic pathways to NHC ligated metal complexes.

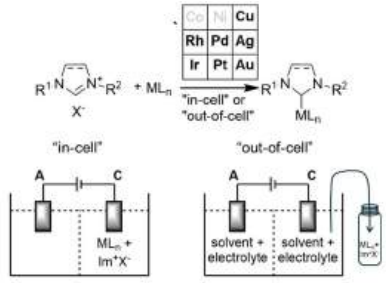

Figure 2. Electrochemical methods developed

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CCS - D1 - F03
Biomass-based monomers for recyclable polymers: A pathway toward sustainable chemistry

Rebecca Sebers[1], Leon Klug[1], Justus Kümper[1], Moritz Haus, Andrij Pich[2], Regina Palkovits[1]
[1]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Germany; [2]DWI – Leibniz Institute for Interactive Materials, Germany

Functional polymers are key enablers of modern technologies, providing targeted performance in applications such as detergents, cleaning formulations, paper processing, textiles, cosmetics, and pharmaceuticals, often at very low dosages. Their functionality, ranging from dispersing and thickening to adsorption and stabilization, is intrinsically linked to polymer structure and monomer selection. However, most state-of-the-art functional polymers are still derived from fossil resources and exhibit limited end-of-life options, highlighting the urgent need for sustainable chemical solutions.[1]

In response to this challenge, our research focuses on catalyzed pathways toward biobased monomers and polymers that combine high performance with improved environmental compatibility. Central to this approach is the utilization of renewable feedstocks and catalytic transformations that enable the design of recyclable and biodegradable functional polymers. Examples include the catalytic hydrogenolysis of sugar alcohols such as sorbitol over mixed metal oxides (e.g., CaZrO), yielding ethylene glycol and 1,2-propylene glycol with selectivities of up to 50%[2], as well as electrochemical routes for converting amino acid derivatives into functional monomers, exemplified by the synthesis of acrylonitrile from glutamic acid.[3] Furthermore, the catalytic conversion of biobased succinic acid into N-vinyl-2-pyrrolidone demonstrates the potential of renewable C4 building blocks for high-value specialty monomers, supported by favorable life-cycle assessment results.[4]

Building on these advances in sustainable monomer synthesis, we recently developed novel biobased amphiphilic polyesters as functional polymer alternatives to fossil-based dispersants such as polyacrylic acid. The resulting polymers are water-soluble, exhibit excellent dispersing performance in hard-water systems, and surpass conventional benchmarks under demanding conditions, while remaining enzymatically degradable.[5]

Overall, this work illustrates how catalysis-driven monomer synthesis and polymer design can be integrated to deliver new chemistry solutions for sustainable functional polymers. By combining renewable feedstocks, efficient catalytic transformations, and end-of-life considerations, these approaches contribute to closing material cycles and advancing the transition toward a circular polymer economy.

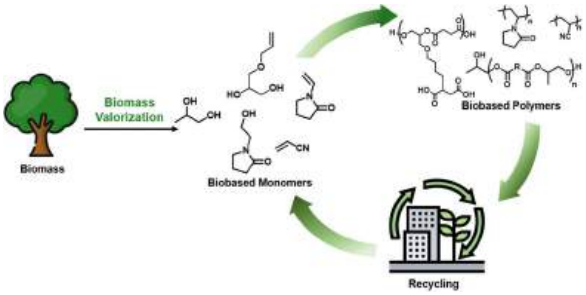

Fig. 1. Schematic representation of the development of Circular Economy for biomass-based functional monomers.

This work was supported by the Werner Siemens Stiftung (WSS, catalaix Project).

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CCS - D1 - F04

Upscaling nanocellulose in catalysis with novel in-flow applications for amino- and metal-driven reactions

Elisa Giovanna Faggioli[1], Aref Rezaei[1], Carlo Punta[1,2], Alessandro Sacchetti[1,2]
[1]Politecnico di Milano, Italy; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy

Amino-catalysed reactions continuously attract great interest in organic synthesis, both for guaranteeing basic environments and for chelating properties towards metals that amino-derivatives show. However, a current issue is the use of amine-containing molecules as homogeneous organocatalysts, implying complex separation steps and high amounts of waste, against the growing request of greener and more sustainable processes. In turn, state-of-art heterogeneous catalysts are designed with green purposes in mind, aiming at easier recovery, biodegradability and recyclability of all materials[1]. In this context, the use of biopolymers as heterogeneous supports represents a promising option, as they complement their renowned environmentally friendly characteristics with great structural flexibility[2]. Cellulose and its nano-derivatives have already been investigated as scaffolds for nanoparticles (NPs), a widespread method to perform metal-catalysed reactions in chemical engineering[3]. NPs offer several advantages, such as high surface area and ease of access for reagents, but they suffer from slower reactivity with respect to their homogeneous counterparts.

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To overcome these issues, in this work we first extracted cellulose nanofibers (CNFs) with chemical (TEMPO-oxidation) and mechanical methods (obtaining TOCNFs), and we functionalised them with amino groups (Fig. 1), developing an engineered nanocellulose material with dual ability: by itself, for amino-catalysed reactions, and as a coordinating agent for transition metal ions. In this way, we were able to turn an inert polymeric scaffold into an active participant in Knoevenagel condensations (Fig. 2a) and click reactions (Fig. 2b). The reactivity of our homogeneous-inspired heterogeneous catalysts in powder form was promising, with excellent yields in flow-mode, gram-scale laboratory settings. Current developments include the production of other catalytic materials, such as membranes, to expand the reactivity scope and accelerate the scale-up of our novel nanocellulose-based catalysts.

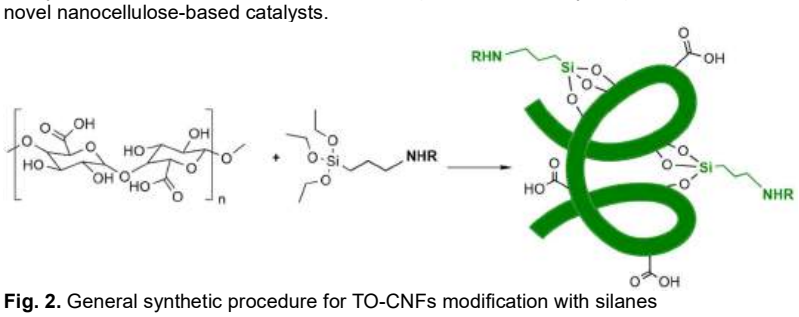

Fig. 2. General synthetic procedure for TO-CNFs modification with silanes

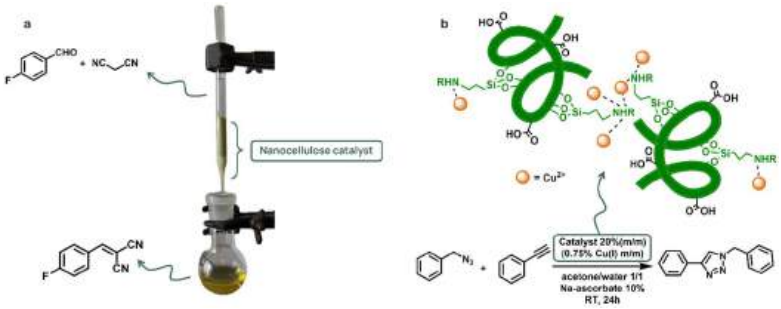

Fig. 3. a) gram-scale, flow-mode setup for lab synthesis of Knoevenagel condensation products with powder amino-modified TO-CNFs; b) General synthesis for click reaction products with metal-coordinating TO-CNFs with Cu^{2+} ions

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CCS - D1 - F05
Dual-active-site in Pt-Co/Z-HP catalyst via strong metal-support interactions for VOCs oxidation

Hui Xu[1]
[1]FuDan University, China

A Pt-Co/Z-HP catalyst with strong metal–support interaction (SMSI) was developed for efficient room-temperature formaldehyde (HCHO) oxidation. The catalyst exhibits highly dispersed Pt nanoparticles, abundant surface hydroxyl groups, and a defect-rich nitrogen-doped carbon matrix. These features promote Pt stabilization, oxygen activation, and intermediate conversion, achieving nearly 100% HCHO removal and CO_2 selectivity under ambient conditions. Density functional theory (DFT) calculations further reveal that plasma-induced –OH species regulate the surface coverage of active hydroxyls, maintaining a balance between O_2 activation and HCHO adsorption. Moreover, comparative models of isolated Co and Pt clusters (Conp–Ptnp–NC) and Pt–Co alloy clusters (CoPtnp–NC) demonstrate that the alloy structure achieves lower reaction barriers for both O_2 dissociation and HCHO oxidation via synergistic dual-site cooperation. These findings highlight that appropriate –OH coverage and Pt–Co electronic synergy are critical for enhancing catalytic performance. This work provides a low-energy approach for designing advanced volatile organic compounds (VOCs) oxidation catalysts via tailored SMSI.

This work was supported by the Shanghai Environmental Science and Technology Project of China (Grant No. [2025], “Demonstration of Cooking Fume Odor Control Technology Based on Adsorptive Material Modification and Evaluation of Its Effectiveness in Typical Application Scenarios”).

CCS - D2 - O01

A carbon-free incipient wet impregnation strategy for vanadium catalysts: Stability modulation on silicalite-1 in oxidative and non-oxidative propane dehydrogenation

Jose Alirio Mendoza Mesa[1], Iqtidar Ali Khan[1], Run Zou[1], Giovanni Pampararo[1], Juan Sebastian Mendoza Paez[2], Michiel Dusselier[1]
[1]Ku Leuven, Belgium; [2]University of Hohenheim, Germany

A novel carbon-free incipient wetness impregnation (IWI^{CF}) strategy is presented as a versatile platform to control vanadium dispersion beyond conventional preparation methods. This approach enables targeted bimetallic deposition and re-dispersion, relocating vanadium species to specific positions within the catalyst crystal and across the support architecture. A mechanistic framework describes how the new complexing agent governs vanadium speciation, transport, and redistribution, providing a rational basis for designing vanadium-based catalytic materials.
Propane dehydrogenation under non-oxidative(PDH) and oxidative (OPDH) conditions[1,2], was used to evaluate catalytic performance. IWI^{CF}-prepared catalysts exhibited comparable or slightly enhanced activity relative to a conventional incipient wetness reference. Compared with the other materials tested, Silicalite-1-based catalysts showed the highest activity and stable selectivity, achieving 41% propane conversion with 90% propylene selectivity under steady-state conditions.
An integrated analysis comprising regeneration–cyclability testing, in situ mass-spectrometric coke characterization, , and activity–deactivation mapping box-plot catalytic profiling reveals experimental evidence for a bimolecular pathway involving C_6 hydrocarbon intermediates[3]. There, surface-confined propylene undergoes secondary C–C coupling, forming adsorbed C_6 olefinic intermediates that act as collateral reaction precursors(coke and cracking). This mechanism explains the high activity and subsequent resistance to deactivation via carbon accumulation on silicalite-1. Remarkably, CO_2 further contributes beyond simple coke mitigation via the Boudouard reaction, competing with propylene for adsorption, reducing residence times of reactive intermediates, and enhancing catalytic stability under OPDH relative to PDH.

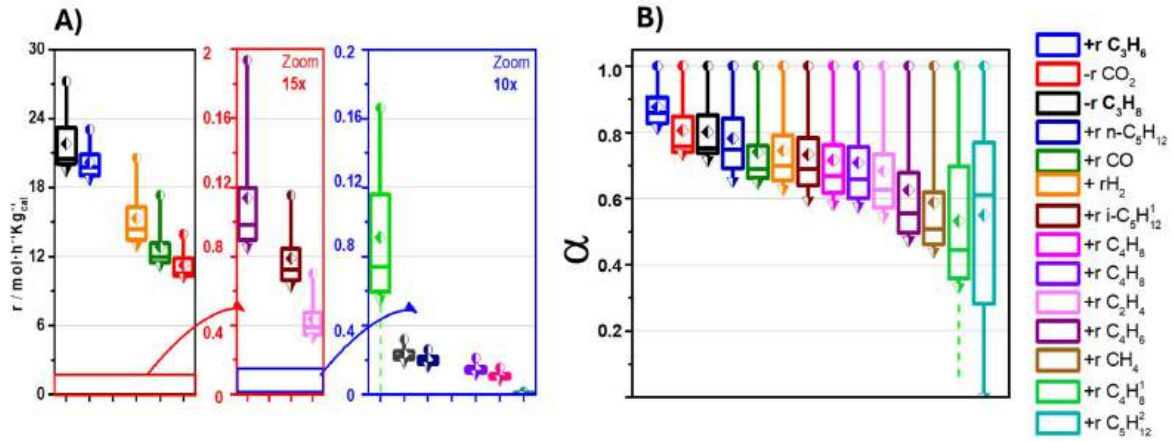

Figure 1. a) ***Activity mapping*** of reactant and product rates (median-sorted). **b)** ***Deactivation mapping*** of reactant and product relative activity (sorted by final median values). **Reaction conditions:** 600 °C, 1 bar, 100 mg S1 catalyst (1.3 mmol V/g, 125–250 µm), $CO_2/C_3H_8/N_2$ = 2.5/2.5/5 Nml min^{-1}, GHSV = 3.0 × 10^3 Nml gas ml^{-1} cat h^{-1}, WHSV = 0.5 g C_3H_8 g^{-1} cat h^{-1}, 10 cycles × 100 min, regeneration in air 10 Nml min^{-1}. **Box-and-whisker analysis:** (quartile = 25 min) and stage 11 at 1500 min (quartile = 375 min). Superscripts in the labels indicate structural isomers. Although GC did not detect C_6 species, statistical correlations between C_1 + C_5 and C_2 + C_4 product distributions support the presence of C_6 intermediates in adsorbed states.

Overall, IWI^{CF} establishes new synthesis variables that modulate metal–support interactions while providing environmental, practical, and economic benefits for vanadium-based catalysts. When coupled with box-plot activity–deactivation mapping, this methodology bridges clean-material synthesis and data-centric catalytic analysis and delivers mechanistic insight into CO_2 valorisation through OPDH. The research strategy presented in this work enables simplified yet information-dense catalytic profiling aligned with emerging machine-learning and artificial-intelligence frameworks for sustainable applications.

This work was performed in the framework of the Moonshot clusterSBO project D2M2 (HBC.2022.0538) “Dioxide-to-Monoxide Bis: Innovative catalysis for CO2 to CO Conversion”), with the financial support of VLAIO (Flemish Agency for Innovation and Entrepreneurship) via the Flemish spearhead cluster Catalisti. D$_2$M^2 is the main funding.

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CCS - D2 - O02
Electro- and photocatalytic ammonia oxidation with RuBda-functionalised carbon materials

Jan Holub[1]
[1]*University of Chemistry and Technology, Prague (UCT, Prague), Czech Republic*

Transitioning from fossil fuels to sustainable alternatives will require diversification across multiple energy sources. Molecular hydrogen is widely regarded as a key candidate; however, its production via water oxidation is highly energy-demanding (1.23 V vs NHE, 180 MJ per kg H_2)[1], limiting future green production to regions with year-round access to cheap renewable energy. As with fossil fuels, the rest of the world will have to depend on H_2 transportation and redistribution. A possible solution could lie in the employment of an inexpensive, easily transportable hydrogen carrier. Recently, ammonia has emerged as a strong contender due to its high hydrogen density (1.9× E/l of liquid H_2)[1], favourable splitting thermodynamics (–0.092 V vs NHE, 33 MJ per kg H_2)[1], existing global logistics, and superior safety compared to liquefied hydrogen.
Electrocatalytic ammonia oxidation (AO) yields inert byproducts (N_2, NO_3^-, H^+/H_2), thereby avoiding the formation of explosive mixtures (unlike water oxidation, which yields O_2 and H^+/H_2). This trait enables single-compartment operations, thereby further simplifying related electro- and photocatalytic approaches and setups.
Here, we would like to report on ammonia oxidation using hybrid molecularly functionalised heterogeneous systems. Specifically, we investigated the activity of RuBda-functionalized carbon paper electrodes (Bda = 2,2′-bipyridine-6,6′-dicarboxylic acid)[3] and developed a novel RuBda/C_3N_4-based hybrid photocatalyst. Our system employs carbon nitride as a photosensitiser and ruthenium complex as the catalytic centre for ammonia oxidation, providing an efficient platform for photocatalytic NH_3 decomposition into N_2 and H^+. Our relatively simple systems offer novel ways to utilise hybrid catalytic systems for sustainable energy conversion and, potentially, wastewater treatment, as well as expanding the range of alternatives to conventional hydrogen production.

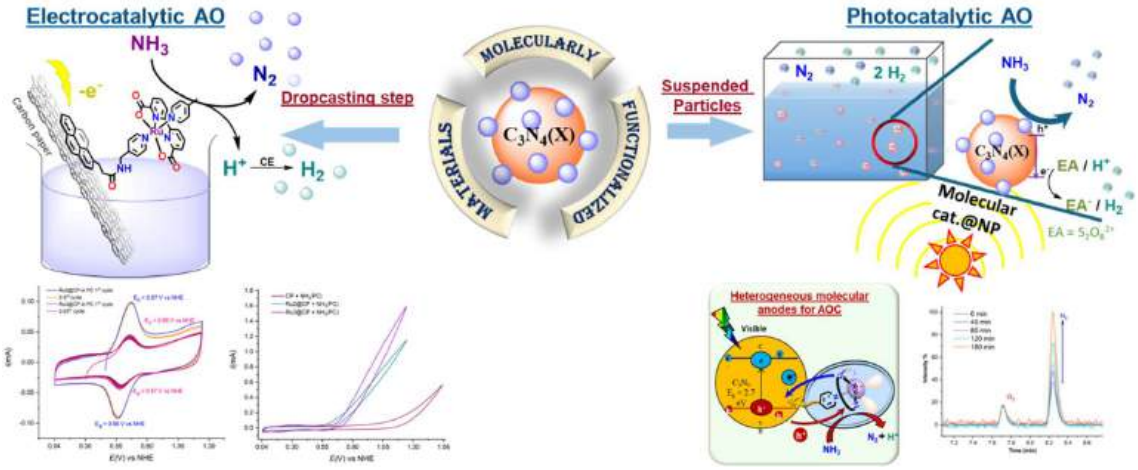

Fig. 1. Illustration of electro- and photocatalytic approach towards ammonia oxidation (AO)

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CCS - D2 - O03

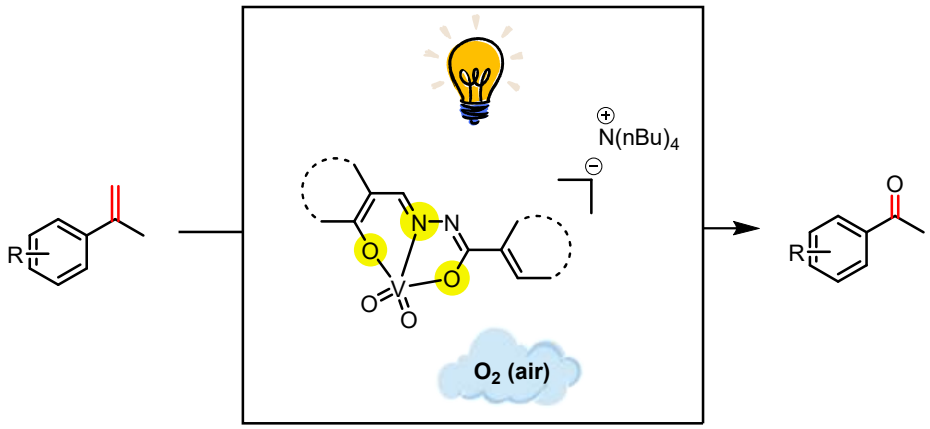
Dioxo-vanadium(V) ONO complexes for aerobic photocatalytic cleavage of C=C bonds

Maria Antonietta Di Stefano[1], Maria Edith Casacchia[1], Sara Sciarretta[1], Massimiliano Aschi, Marcello Crucianelli[1], Andrea Di Giuseppe*[1]

[1]*Dept. of Physical and Chemical Sciences, University of L'Aquila, Italy*

Selective oxidative cleavage of C=C double bonds is a key transformation to introduce oxygen functionalities into organic molecules. Traditional methods present several safety issues due to the use of toxic, unstable oxidants, the generation of stoichiometric waste, and the requirement for harsh conditions.[1] To date, all reported vanadium-catalysed oxidative cleavage reactions require a stoichiometric amount of hazardous oxidant as the oxygen source.[2]

Herein we present novel dioxo-vanadium(V) complexes with O-N-O pincer ligands derived from Schiff bases able to catalyze the photocatalytic oxidative cleavage of C=C bonds under mild reaction conditions using air as the only oxygen source without further additives. Vanadium was selected as the central metal due to its ability to access multiple oxidation states, for its natural abundance, and for its relatively low cost.[3] The photocatalytic efficiency of these new vanadium-based complexes was evaluated by performing photocatalytic oxidative cleavage of styrenes in presence of air. Mechanistic investigation, supported by DFT calculations, indicate that a ligand-to-metal charge transfer (LMCT) excited state is generated *via* photoexcitation, which promotes both substrate activation and oxygen incorporation.



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CCS - D2 - O04

Engineering 2D semiconductor heterojunctions for efficient visible-light-driven photocatalysis toward sustainable chemical conversions

Onder Metin*, Melek Sermin Ozer, Zafer Eroglu, Ayman Batuhan Ayyıldız, Aleyna Basak
Dept. of Chemistry, College of Sciences, Koç University, Türkiye

Human progress in areas such as agriculture, energy, and medicine has significantly enhanced comfort of life, while generating serious environmental issues. Addressing these issues has made sustainability a defining challenge of our time. Chemistry is central to this effort, as virtually all industrial products and technologies depend on chemical transformations. In response, green chemistry has emerged as a guiding framework for redesigning chemical processes to be safer, cleaner, and more efficient. A key strategy within this framework is the use of light-driven catalytic systems that can utilize abundant solar energy to promote chemical reactions. Semiconductor-based photocatalysts have been extensively studied for a wide range of chemical transformations. Despite their potential, many conventional semiconductors suffer from intrinsic limitations, including unsuitable energy-band structures and rapid recombination of photogenerated electrons/holes. To overcome these issues, researchers have developed several approaches such as reducing materials to nanoscale, hetero-atom doping, and combining with different semiconductors to form heterojunctions. In particular, few-layer 2D semiconductors have attracted strong interest due to their unique electronic and surface properties, but many 2D materials suffer from weak absorption in the visible region and inefficient charge utilization.

High-performance photocatalysts must be able to absorb visible-light effectively and convert the resulting excited charges into useful chemical reactivity before recombination. Creating heterojunctions between different semiconductors has proven to be a powerful solution, because the interfaces formed between distinct materials generate internal electric fields that drive electrons and holes in opposite directions. This spatial separation greatly extends the lifetime of charge carriers and increases the probability that they participate in surface reactions.

Here, I will talk about our recent studies on rational design of 2D semiconductors-based heterojunction photocatalysts for visible-light-driven sustainable chemical transformations including photoredox C–H functionalization, photooxidation and hydrogen peroxide production. The authors thanks to TUBITAK for the financial support (Grant No: 123056).

CCS - D2 - O05
A versatile family of [IrCp*Cl(N^O)] (photo)catalysts: Unlocking new challenging reactivities

Andrea Uroz[1], Laura Blanco[2], Kevin Gutiérrez[2], Alba Collado[2,3], Silvia Cabrera[2,3], José Alemán[1,3]
[1]Organic Chemistry Dept., Universidad Autónoma de Madrid (UAM), Spain; [2]Inorganic Chemistry Dept., UAM, Spain; [3]Institute of Advanced Research in Chemical Sciences (IAdChem), UAM, Spain

IrCp*-complexes have stood up as excellent catalysts for a wide range of organic transformations including C-H activation and hydrogenation. However, their application in photocatalysis remains scarce and examples combining both reactivities are still lacking.[1] Consequently, the development of new Ir-based systems capable of exhibiting dual activity remains a challenge.
In this context we have developed a distinctive family of IrCp*-complexes bearing substituted 8-oxyquinolines ligands (N^O) specifically designed to tune their catalytic properties.[2] These [IrCp*Cl(N^O)] complexes are photoactive in dehalogenation of aromatic halides and in alkenes isomerization, while also acting as efficient catalysts in transfer hydrogenation. Remarkably, both reactivities can be merged into a dual tandem reaction, in which a single IrCp*-complex promotes photo-debromination followed by transfer hydrogenation (Figure 1A). This has been achieved due to their unique ability to go through ligand substitution, unlocking new reactivities not accessible using typical [Ir(ppy)$_3$]. Beyond this, we have developed the diastereoselective photo-polyoxidation of 8-hydroxyquinolines using an *insitu*-formed IrCp* catalyst and air as oxidant. Starting from a catalytic amount of [IrCp*Cl$_2$]$_2$ and 8-hydroxyquinoline as the substrate, the active [IrCp*Cl(N^O)] species plays a dual role by photoactivating O_2 and simultaneously activating the substrate toward selective oxidation (Figure 1B).
The unprecedented combination of reactivities exhibited by these [IrCp*Cl(N^O)] complexes highlights the important role of catalyst design and structure-activity studies. Modulating the photophysical properties of these complexes allows for the development of a broad and versatile catalysts toolbox.

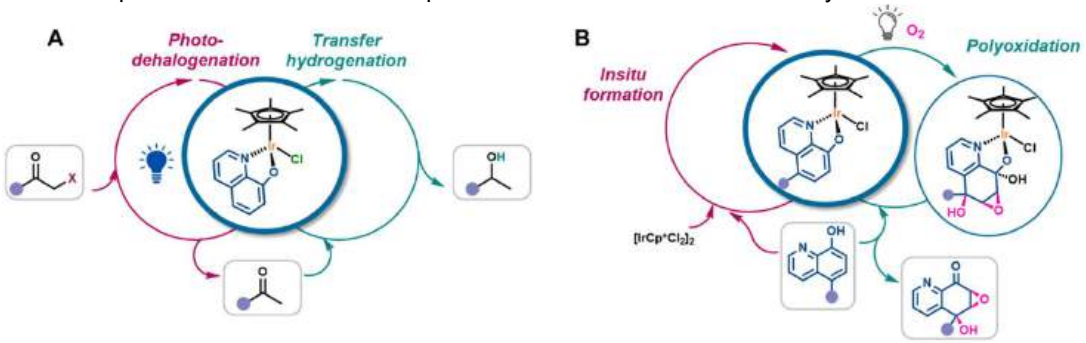

Fig. 1. [IrCp*Cl(N^O)] complexes used in a) dual tadem reaction and b) photo-polyoxidation of 8-hydroxyquinolines.

Acknowledgments: Financial support was provided by the Spanish Government (PID2021-122299NB-100,TED2021-130470B-100,CN2022-135687,PID2024-155520NB-I00,TEC2024/TEC-308),"Proyectos sinérgicos I+D"(Y2020/NMT6469). A.U. thanks MICIU for her predoctoral fellowship.

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CCS - D2 - O06

Photocatalytic Cu-BTC@Fe-MIL-101-NH_2 composite for CO_2 capture and conversion: Advancing greener synthesis and sustainable resource recovery

Ting Yu Chen[1], Kuo-Pin Yu[1*]
[1]Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taiwan

N,N-Dimethylformamide (DMF) is a widely used solvent in chemical synthesis but poses environmental and health risks due to its volatility, persistence, and toxicity. Replacing DMF with N,N-diethylformamide (DEF) offers a greener alternative with lower toxicity, better biodegradability, and reduced volatility. Meanwhile, carbon dioxide (CO_2), the main anthropogenic greenhouse gas, is also a crucial feedstock in urea synthesis, reacting with ammonia under thermochemically extreme conditions. Ammonia production via the Haber–Bosch process (high temperature and high pressure) is energy-intensive and fossil fuel–dependent, leading to significant carbon emissions. These challenges highlight the need for greener synthesis and sustainable resource recovery strategies to minimize the environmental impact of chemical manufacturing.

In this study, we developed a novel composite metal–organic framework (MOF) derived material, Cu-BTC@Fe-MIL-101-NH_2, as a photocatalyst capable of simultaneously capturing CO_2 and reducing nitrate under ambient conditions. This dual-function approach offers a sustainable strategy for mitigating harmful gas accumulation indoors and transforming pollutants into value-added nitrogen-based products. This solar-driven approach directly addresses key bottlenecks in sustainable fertilizer production by integrating CO_2 valorization with nitrogen-pollutant upgrading, thereby advancing circularity in both carbon and nitrogen cycles.

The composite MOF leverages the synergistic properties of Cu-BTC and Fe-MIL-101-NH_2, which provide high surface area, tunable porosity, and abundant active sites for gas adsorption and conversion. A green chemistry route was employed in the synthesis, substituting the hazardous solvent N, N-dimethylformamide with the less toxic N, N-diethylformamide, thereby minimizing health risks during material preparation and reducing environmental burdens. Through structural and mechanistic studies (XRD, SEM, TEM, PL, UV-Vis, EIS, FTIR, XPS) combined with density functional theory simulations, we demonstrate that under visible-light irradiation, the optimized composite achieves high conversion yields of ammonia and urea. These results highlight the material's potential as a next-generation technology for improving net-zero fertilization while advancing sustainable chemical practices.

Keywords: Carbon dioxide; Metal–organic frameworks (MOFs); Photocatalysis

CCS - D2 - O07
Electron transfer reactivity of ion-radical photocatalysts

Kirk S. Schanze[1]
[1]*University of Texas at San Antonio, USA*

There has been recent increased interest in the excited state properties and electron transfer reactions of doublet excited states of ion radicals. This interest is driven in part by the recognition that excited states of anion and cation radicals can serve as "super-reductants" and "super-oxidants" in photocatalytic schemes with difficult to oxidize or reduce substrates as shown in the Figure.[i] This concept has been used in conPET photocatalytic schemes, where the excited state of an anion radical serves as a powerful reducing agent.[ii] In principle, through careful design of ion-radical chromophores it is possible to attain super-redox sensitizers with excited state potentials as positive as E(*+/0) = +3.0 or as negative as E(*-/0) = -3.0 V vs. SCE. Given their powerful redox reactivity, ion-radical sensitizers are thermodynamically capable of driving important redox reactions in solar conversion (e.g., CO2 reduction or water oxidation).

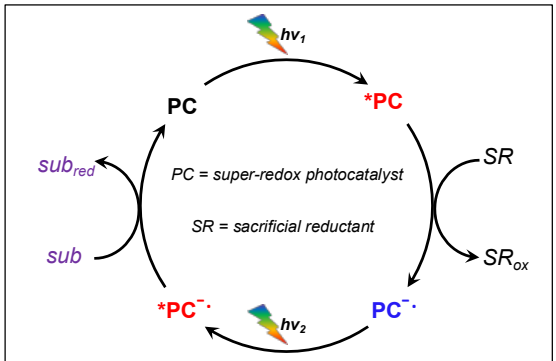

Figure 1. Photocatalytic cycle involving an anion radical doublet excited state (*PC⁻·) as a reducing agent.

We recently demonstrated reduction of difficult to reduce aryl halides by the diffusion-controlled reduction by the excited state of perylene and naphthalene diimide anion radicals, which have E(*-/0) = -1.8 V and -2.1 V vs. SCE, respectively.[iii,iv] The talk will highlight recent results concerning the excited states of ion radicals of a variety of structures, including imides and diimides, organic conjugated heterocycles and oligomer systems. In some cases the doublet excited states of the ion radicals are fluorescent and have lifetimes greater than 500 ps. Factors that control the lifetime of the doublet excited state ion radicals will be discussed.

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CCS - D2 - O08
Light-responsive dynamic covalent systems: Out-of-equilibrium states, switching and catalysis

Petr Kovaříček[1]
[1]*University of Chemistry and Technology Prague, Czech Republic*

Dynamic covalent bonds allow structural adaptation of molecules, thus creating a network of intertwined reactions and constituting a whole chemical system. Such adaptations can occur either spontaneously or can be driven by external stimuli. The range of such stimuli includes thermal, chemical, electrochemical or photochemical ones. Light is one of the most powerful stimuli, largely exceeding thermal excitation and can deliver out-of-equilibrium states corresponding to temperatures up to 500 °C, which is far beyond the decomposition temperatures of organic molecules.[1] Light can also induce intramolecular structural adaptation, such as in the case of photoswitching. In the particular case of acylhydrazone photoswitches featuring a thiophene ring substituted in position 2, the photoswitching is associated not only with a geometrical change, but surprisingly also by switching of the electronic ground state from closed-shell singlet to stable open-shell triplet state. This behavior is also observed in solid state and the diradical character of the triplet isomer can be used as an initiator/catalyst in common radical substitution reactions.[2] The strong out-of-equilibrium shift of photoexcited states and the structural adaptability allows us to expand the concept even further. We have prepared and studied a series of deazaoxaflavins (DAOFs), covalently dynamic analogues of known flavin photocatalysts. DAOFs are potent photoredox catalysts of benchmark reactions and their synthesis is done by two reversible condensation reactions. Upon mixing, dynamic reaction network is established with various concentrations of all species. When photocatalytic conditions are installed, the species able to catalyze is involved in the catalytic cycle and thus removed from the equilibrium. The system responds by producing more of the catalyst due to Le Chatelier principle. As a result, the catalyst formation is driven by its photocatalytic function, a phenomenon of intriguing importance in the field of catalysis.[3]

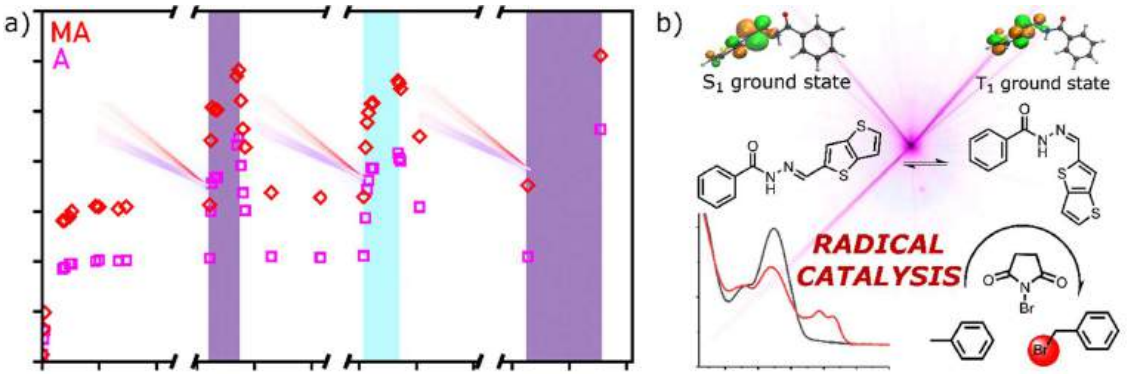

Figure 2a) out-of-equilibrium composition of dynamic chemical systems. b) electronic ground state photoswitching.

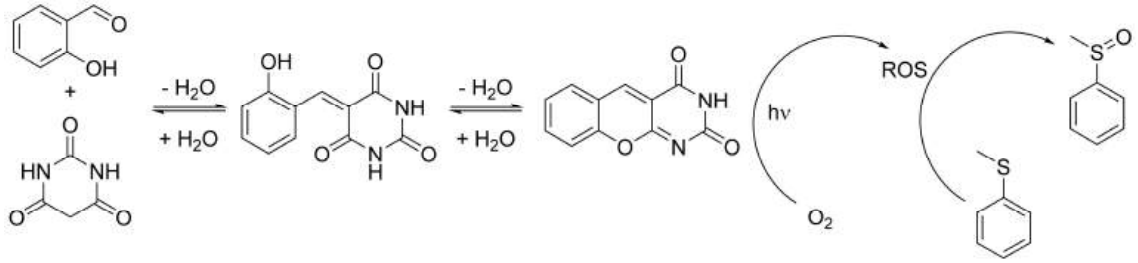

Fig. 3. Fully reversible pathway generating light-responsive chemical network yielding potent photoredox catalysts, formation of which is driven by their photocatalytic function.

This work was funded by the Czech Science Foundation grant JuniorSTAR 22-11299M.

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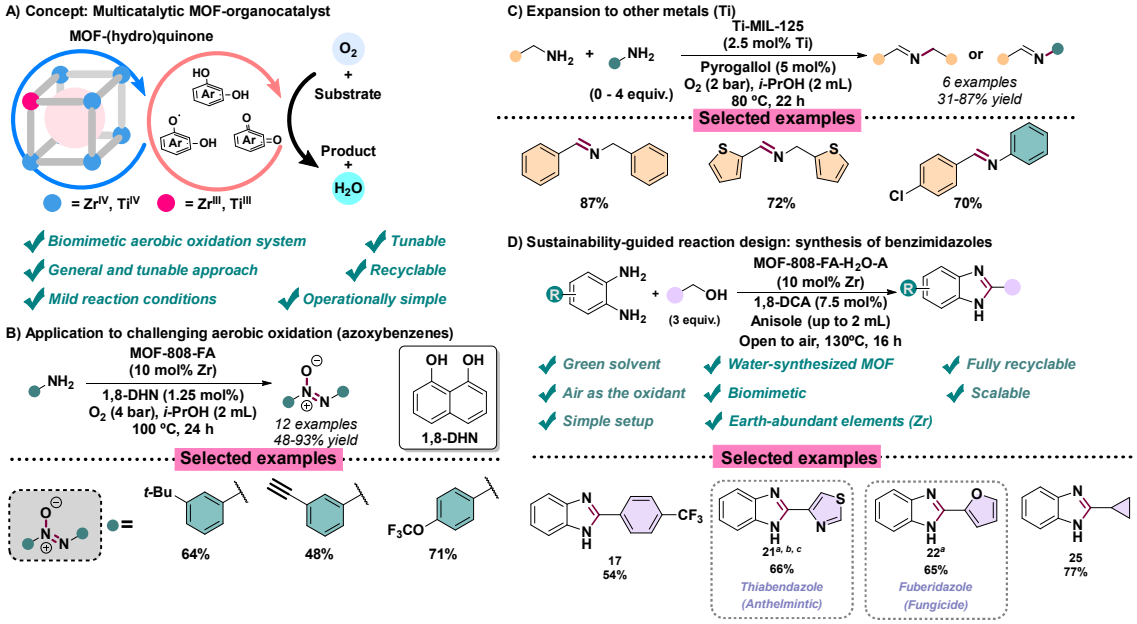
CCS - D2 - O09
Biomimetic MOF-based multicatalytic systems for green aerobic oxidations

Miguel A. Rivero-Crespo[1,2]
[1]Dept. of Chemistry, Stockholm University, Sweden; [2]Wallenberg Initiative Materials Science for Sustainability, Sweden

Molecular oxygen (O_2) is an ideal sustainable oxidant, but achieving high selectivity in aerobic oxidation reactions remains a significant challenge often requiring noble metals, high pressures or light activation. We have developed a novel biomimetic multicatalytic strategy that combines earth-abundant metal-organic frameworks (Zr/Ti-MOFs) with commercially available (hydro)quinone-type organic cocatalysts (Fig. 1A).[1] This **MOF–organocatalyst system** enables the selective aerobic oxidation of anilines to azoxybenzenes, a historically elusive transformation, under mild conditions with excellent yields and selectivities (Fig. 1B).
The cooperative interplay between the cocatalyst and the MOF triggers an electron transfer at the Zr-oxo nodes, transforming redox inactive Zr^{IV} into open-shell Zr^{III}, able to activate O_2 and generate reactive oxygen species (ROS) in the dark. The proximity of active sites allows efficient trapping of highly reactive intermediates, steering the reaction toward the azoxybenzene products and suppressing side reactions. Notably, this cooperative catalysis is achieved **without any post-synthetic modification** of the MOF, highlighting the power of simply pairing off-the-shelf MOFs with organic redox mediators to unlock new reactivity.
The approach is highly tunable and general. We demonstrate its extension to the oxidative dimerization of thiols by simply changing the cocatalyst and even expand it to a Ti-based MOF (MIL-125) to accomplish the aerobic oxidative coupling of amines (Fig. 1C), underscoring the broad potential of the MOF–cocatalyst concept. Finally, we have applied this concept to **sustainability-guided reaction design** achieving the synthesis of benzimidazoles by aerobic oxidation that addresses common drawbacks of previous methods (Fig. 1D). Overall, this work showcases a **conceptual innovation** in MOF catalysis: a modular platform that harness the power of multicatalysis, opening new avenues for designing challenging reactions under environmentally benign conditions.

Fig. 1.



[1]Arango-Daza, J. C.; … Rivero-Crespo, M. A. *Angew. Chem. Int. Ed.* **2026**, 65, e23426.
[2] Arango-Daza, J. C.; … Rivero-Crespo, M. A. *unpublished*.

CCS - D2 - O10

Toward robust and scalable formulation of ceramic-supported catalysts for reversible hydrogen storage using LOHCs

Limor Ben Neon[1*], Betsy Kurisingal Joseph[2], Issam Nciri[2], Karine De Oliveira Vigier[2], Christophe Coutanceau[2], Mikhael Bechelany,[1] Martin Drobek[1], Anne Julbe[1*]

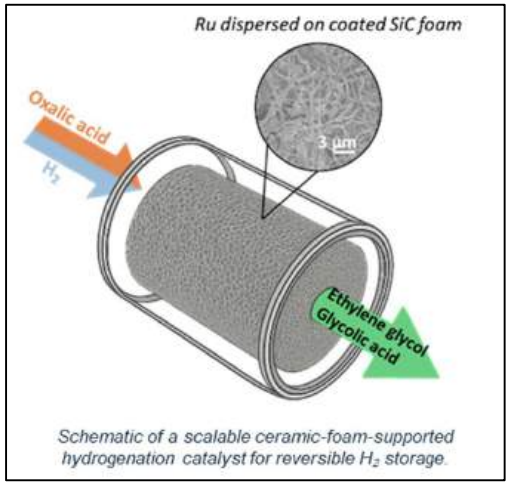
[1]Institut Européen des Membranes (IEM); CNRS, ENSCM, Univ Montpellier; France; [2]Institut de Chimie Des Milieux et Des Matériaux de Poitiers (IC2MP), Université de Poitiers, UMR 7285 CNRS, France

The transition to a hydrogen-based energy economy demands safe, efficient, and scalable hydrogen storage solutions. Liquid Organic Hydrogen Carriers (LOHCs), such as ethylene glycol, offer a promising route for reversible hydrogen storage under mild conditions. Within the French-funded BHyoLOHC project, our research focuses on advancing catalytic technologies for LOHC systems, emphasizing sustainability and innovative materials.

At the Institut Européen des Membranes (IEM), we are developing robust ceramic-supported catalysts for the hydrogenation of oxalic acid to ethylene glycol—a key reaction enabling hydrogen storage. Our primary goal is to enhance the scalability of reversible H_2 storage by integrating Ru-based catalysts on ceramic foams. In collaboration with IC2MP, these catalytic systems are evaluated under continuous flow to assess activity, selectivity, and stability under realistic operating conditions.

We leverage microwave-assisted synthesis to produce highly active catalysts on ceramic foams.[1,2] This approach offers multiple advantages: shorter synthesis times, improved energy efficiency, use of green solvents, easier catalyst handling, and access to novel physicochemical properties unattainable via conventional thermal methods. These properties arise from microwave/matter interactions and the differing dielectric loss constants of liquids and solids, which we exploit to generate ultra-highly reactive microenvironments at these interfaces. Leveraging this effect, we developed two distinct methods: (i) formation of stabilized, highly porous θ-alumina catalyst carriers supported on ceramic foams,[1] and (ii) dispersion of transition metal particles on graphene-coated ceramic foams.

This presentation will showcase our microwave-assisted synthesis strategies, benchmark catalytic performance, and discuss the potential of these materials for next-generation LOHC-based hydrogen storage. By combining advanced synthesis techniques with sustainable materials engineering, our work contributes to the broader development of efficient, environmentally responsible hydrogen storage systems, supporting global decarbonization objectives.



Schematic of a scalable ceramic-foam-supported hydrogenation catalyst for reversible H_2 storage.

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CCS - D2 - O11
Probing nanozymatic activity in metal-organic frameworks via luminescent Linkers

Maxim Lox, Tatjana N. Parac-Vogt
KU Leuven, Belgium

Metal–organic frameworks (MOFs) are crystalline materials composed of inorganic nodes and organic linkers, offering high porosity and tunable surfaces. Their modularity has enabled biomolecule-compatible applications such as catalysis and drug delivery.[1] Several Zr-based MOFs, including UiO-66[3] and MOF-808,[4] promote peptide bond hydrolysis and function as artificial proteases or nanozymes.
Despite these advances, the molecular mechanisms governing MOF-mediated proteolysis remain poorly understood. Protein adsorption, conformational rearrangement, and exposure of labile peptide bonds are often inferred rather than directly probed. Moreover, most studies emphasize material optimization rather than how intrinsic protein properties, such as charge distribution or hydrophobicity, control adsorption and cleavage selectivity. Understanding these interfacial processes is essential for the rational design of selective MOF nanozymes.
Here, we examine protein adsorption and hydrolysis on the luminescent Zr-based LMOF-601,[5] whose emissive linkers enable spectroscopic monitoring of interfacial events. Structurally distinct proteins (lysozyme, α-lactalbumin, and myoglobin) were examined. All proteins adsorbed to LMOF-601, yet hydrolysis occurred exclusively for myoglobin, demonstrating that adsorption alone does not predict catalytic susceptibility. Multivariate analysis identified distinct surface-property determinants for adsorption and cleavage, while time-resolved fluorescence indicated hydrophobic-driven binding and partial unfolding of myoglobin, facilitating peptide bond exposure.
These results establish a molecular link between protein-MOF interactions and catalytic outcomes and highlight luminescent MOFs as analytical platforms for studying biointerfaces.

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[3]Swinnen, S.; Lox, M.; de Azambuja, F.; Parac-Vogt, T. N ACS Appl. Nano Mater. **2025**, 8 (7), 3536–3544.
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CCS - D2 - O12

Crystal engineering of zinc metal-organic frameworks with intrinsic dynamicity for multicomponent catalysis

Xu Jia[1], Chongting Ren[1], Shengyun Hu[1], Cui-Lian Liu[1,2]*, Simon Mathew[2], Wim Dehaen[1], Tatjana N. Parac-Vogt[1] and Luc Van Meervelt[1]*

[1]Dept. of Chemistry, KU Leuven, Belgium; [2]Van 't Hoff Institute for Molecular Sciences, Universiteit van Amsterdam, Netherlands

Metal–organic frameworks (MOFs) with molecular-scale tunability provide a customizable platform for efficient organic synthesis.[1] By tailoring both ligands and coordination modes, catalytic sites could be immobilized within a porous framework, while substrates and products traverse the interconnected channels unhindered, offering promise in heterogeneous catalysis. To position MOFs as broadly applicable catalytic materials, it is imperative to conduct a systematic evaluation of their fundamental performance metrics.[2]

Herein, we report a Zn-MOF catalyst endowed with intrinsic dynamic behaviour and introduce a combined strategy of X-ray diffraction crystallography and *ab* initio molecular dynamics (AIMD) to evaluate framework dynamicity during catalysis. (Figure 1) High-throughput analysis of structural data, guided by AIMD, first identifies the flexible and rigid regions of the overall framework. We then probe the dynamic structural evolution under systematically varied temperatures, solvent environments, and substrate identities. Finally, by correlating these dynamic transformations with the performance of a multicomponent coupling reaction, we propose a novel "dynamic steric-adaptation" mechanism that accounts for the observed reactivity enhancements. This integrative approach offers new mechanistic insight into MOF-mediated transformations, and establishes a blueprint for designing dynamically adaptive porous catalysts for advanced organic syntheses.

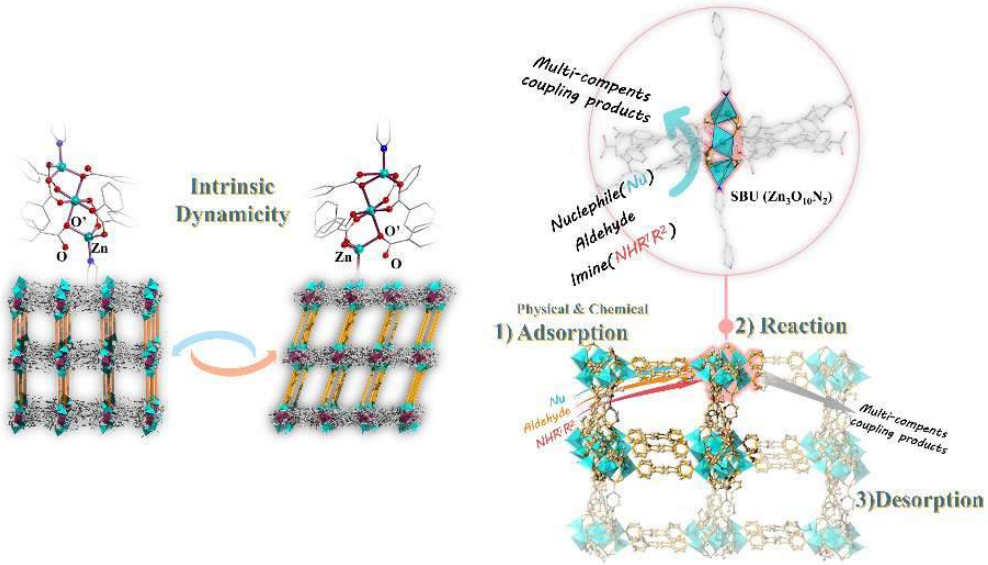

Fig. 1. Framework and node transformations governing the intrinsic dynamicity of the Zn-MOF and its application in multicomponent coupling reactions.

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[2]Pascanu, V.; Miera, G. G.; Inge, A. K.; Martín-Matute, B. *J. Am. Chem. Soc.* **2019**, *141*, 7223–7234.

CCS - D2 - O13
Advancing sustainability via molecular design of nanomaterials

Iván Sorribes[1]
[1]*Institute of Advanced Materials (INAM), Universitat Jaume I, Spain*

Modern society depends on fossil fuels for energy and chemical production, but they are limited resources, and their use contributes to global warming and significant environmental pollution. Key to successfully reduce our fossil fuel overreliance relies on catalysis and, more specifically, on the development of catalysts with exceptional properties. However, discovering methodologies to precisely control the final structure of the catalysts at the nanoscale remains a challenge. This lack of control hinders the design of materials with tailored catalytic properties, as it prevents clear structure–performance relationships.
Transition metal chalcogenides, and particularly MoS_2, have been proposed as promising catalysts to drive the transition from refining to circular and sustainable production of energy and chemicals. However, their performance is intrinsically restrained because of the scarce number of actives sites compared to their available surface area. Therefore, it is very important to establish new synthetic strategies to design their surface with atomic-scale control with the aim of obtaining more accessible active sites of specific nature and location.
This communication will show how an innovative bottom-up synthetic strategy, which employs molecular cluster complexes as precursors, can be used as a reliable tool for the precise engineering of this kind of nanomaterials. The resulting sulphur-deficient and sulphur-enriched molybdenum sulphide nanomaterials, named $\{Mo_3S_{4\text{-}7}\}_n$, preserve the specific atomic arrangement of the molecular cluster motif precursor, a fact that leads to the presence of proliferated structural defects, i.e. active sites, at the naturally occurring edge positions and along the commonly non-active basal planes. This results in multifunctional catalytic platforms that have been successfully applied as heterogeneous catalysts for process intensification in fine chemical synthesis,[1-3] and for the Hydrogen Evolution Reaction (HER).[4] Their versatility in obtaining value-added chemicals and hydrogen through hydrogenation, dehydrogenation, electrocatalytic and photocatalytic reactions will be demonstrated (Figure 1).

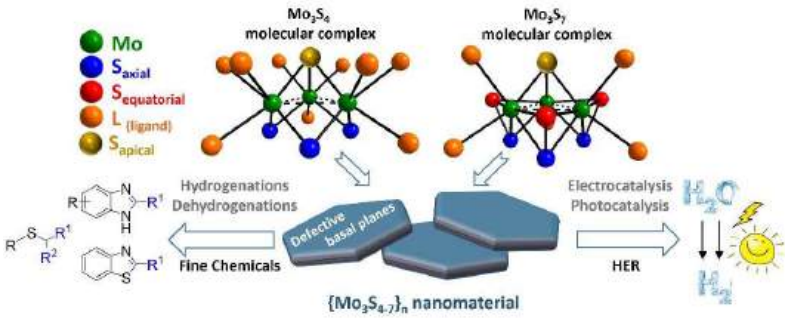

Fig. 1. Schematic representation of nanomaterials $\{Mo_3S_{4\text{-}7}\}_n$ derived from molecular clusters and their application as catalysts for the synthesis of fine chemicals and for the hydrogen evolution reaction.

Acknowledgements: This work has been supported by the Grant PID2022-143164OA-I00 funded by MICIU/AEI/10.13039/501100011033 and by "ERDF/EU", as well as by the Grant CNS2022-136183 funded by MICIU/AEI/10.13039/501100011033 and by "European Union NextGenerationEU/PRTR". The Grant ESGENT/016/2024 funded by the Gen-T Plan of the Generalitat Valenciana is gratefully acknowledged as well.

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[3]Rodenes, M.; Oštrić, D.; Martín, S.; Concepción, P.; Corma, A.; Sorribes, I. *ChemSusChem* **2025**, 18, e202500343.
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CCS - D2 - O14

Catalysis-driven routes to bio-based acetate and acrylate esters: Integrating bioprocessing and enzyme-enabled chemistry

Van Hecke, W., Martinez-Garcia, M., De Wever, H.
Flemish Institute for Technological Research, Belgium

This contribution presents an integrated catalytic roadmap toward acetate- and acrylate-derived esters, combining intensified bioprocessing with lipase-catalyzed chemistry.

Upstream, membrane bioreactor (MBR) technology enables high-productivity, continuous production of acetic and lactic acid from renewable carbon sources. By decoupling biomass retention from hydraulic residence time, MBRs achieve high volumetric productivities. While lactic acid is predominantly valorized via poly(lactic acid), its catalytic dehydration to acrylic acid offers a promising bio-based alternative to the conventional petrochemical propylene route. Acetate is positioned as a flexible C_2 platform molecule, accessible from both sugars and gas-based CO_2/H_2 routes, enabling integration with circular carbon and power-to-chemicals concepts. Conversion of acetate toward acrylic acid remains chemically challenging and an active area of research.

Downstream, acrylic acid is treated as a reactive intermediate rather than a final product, enabling access to value-added ester derivatives. In parallel, acetate esters are important end products with established applications in the flavour, fragrance, solvent, and specialty chemical sectors. Growing demand for renewable feedstocks and sustainable production processes is driving renewed interest in biocatalytic ester synthesis, which offers high selectivity and mild operating conditions.

Enzymatic catalysis enables genuinely new chemistry solutions. Lipases selectively esterify aliphatic hydroxyl groups while leaving aromatic hydroxyls untouched, as demonstrated in the synthesis of dihydroconiferyl acrylates with antioxidant and antistatic properties. Similarly, mild enzymatic conditions allow the synthesis of functional acrylate esters from challenging substrates such as furfuryl alcohols.

Short-chain organic acids strongly inhibit lipases under solvent-free conditions, rendering direct esterification ineffective at high acid concentrations. These insights established transesterification routes, and fed-batch acid dosing as essential design principles.

Overall, this work demonstrates how integrating renewable biological production with catalysis-driven process design enables novel bio-based ester solutions that bridge chemistry and biology beyond drop-in alternatives.

Acknowledgments: Part of this work was financially supported by Flanders Innovation and Entrepreneurship (VLAIO), Belgium through the Catalisti Moonshot project AC2GEN (HBC.2021.0578), and Catalisti project Enzymase.

CCS - D2 - O15
Pt-based zeolites as bifunctional catalysts for polyolefins depolymerisation

Sophie H. van Vreeswijk[1], Simon Zwartkruis[1], Bert M. Weckhuysen[1]
[1]Utrecht University, The Netherlands

The global demand for plastics continues to rise, while there is an increasing need to reduce our reliance on fossil-based feedstocks. Recycling plastics provides an opportunity to recover and reuse the carbon stored in these materials, contributing to a more circular carbon economy. Among the available recycling strategies, chemical recycling offers a promising route to convert waste plastics into valuable hydrocarbons and chemical feedstocks for multiple purposes. Several chemical recycling approaches exist, including pyrolysis, solvolysis, hydrocracking, and hydrogenolysis.
In this work, we combine hydrogenolysis and (hydro)cracking by designing a catalyst system that integrates Pt nanoparticles on an acidic zeolite support. Both medium-pore zeolite ZSM-5 and large-pore zeolite Y are investigated. Pt catalyses hydrogenolysis, while the zeolite framework provides active sites for (hydro)cracking. This bifunctional catalyst material enables efficient and relatively rapid polyethylene depolymerisation at low temperatures (150–250°C), demonstrating enhanced activity compared to single-function systems.
We investigate the effect of the introduction of Pt to the zeolite materials on their acidic, structural, electronical and morphological properties. Additionally, the differences in product distributions obtained from hydrogenolysis and hydrocracking individually are studied, as well as the changes that arise when both processes are combined. The influence of the reaction temperature is also investigated. Hydrogenolysis primarily yields light saturated hydrocarbons, whereas hydrocracking produces a broader range of heavy saturated and aromatic hydrocarbons. By integrating both pathways within a single catalytic system, improved control over product selectivity is achieved, along with faster depolymerization at lower operating temperatures. Figure 1 shows the effect on the composition of the hydrocarbon mixture, showing a faster depolymerisation behaviour due to hydrogenolysis.

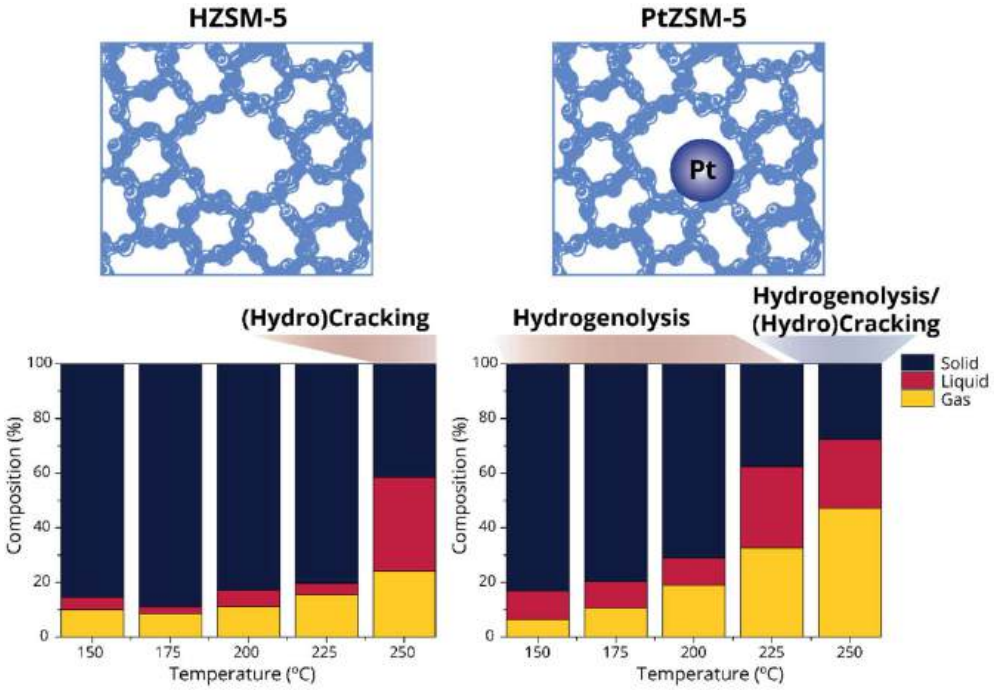

Fig. 1. Composition of the polymer/hydrocarbon mixture after depolymerisation at 200°C with 20 bar H_2 for 2 h showing the difference in depolymerisation temperature with and without Pt on HZSM-5 catalyst.

CCS - D2 - O16
Designing accessible zeolitic materials via solution-phase precipitation

Nelcari-Trinidad Ramírez-Márquez[1], Carlos-Alexander Trujillo[2], Noemi Linares[1], Javier García-Martínez[1]
[1]Laboratorio de Nanotecnología Molecular, Depto de Química Inorgánica, Universidad de Alicante, Alicante, Spain; [2]Laboratorio de Catálisis Heterogénea, Departamento de Química, Facultad de Ciencias, Universidad Nacional de Colombia, Colombia

In the field of zeolite chemistry, partial crystallization emerges as a notable design strategy, offering a distinct approach to decoupling local structural order from long-range crystallinity. The equilibrium of secondary and composite building units (SBUs and CBUs) within disordered matrices has been shown to yield materials with high surface area, strong acidity, and enhanced accessibility. This is particularly relevant for bulky-molecule chemistry [1–3].
In order to generate MFI-derived mesoporous materials enriched in zeolitic building units, two complementary routes are employed. Firstly, hydrothermal crystallization is interrupted (Semicrys_MFI xH), and secondly, soluble silicoaluminate species formed during partial crystallization are precipitated (Prep_MFI xH). These approaches enable direct comparison between solid- and solution-mediated pathways for capturing protozeolitic motifs outside fully crystalline frameworks.
The isotherms of solution-derived materials evidencing significant mesoporosity and high surface area, whereas partially crystallized solids show limited adsorption. Raman spectroscopy has been used to confirm the presence of MFI-related SBUs and CBUs in both solid phases and precipitate. Five-membered ring units have been detected at early crystallization stages. Following the process of precipitation, the locally ordered species are preserved within a disordered mesoporous matrix. This results in a higher contribution of short-range order combined with improved accessibility when compared to partially crystallized solids [2,4].
The materials were evaluated in a series of reactions involving bulky molecules, including Friedel–Crafts alkylation of benzyl alcohol with mesitylene and o-xylene, as well as the cracking of 1,3,5-tri-isopropylbenzene (TiPB). As demonstrated in Figure 2, reactivity escalates with crystallization degree up to an intermediate optimum, before declining as long-range order develops. The maximum activity is observed at intermediate crystallization stages, where SBUs and CBUs provide strong Brønsted acid sites, while excessive framework ordering has limited accessibility. In this regime, the mesoporous matrix facilitates efficient mass transport, whereas more amorphous samples lack sufficient acidity and fully crystalline materials suffer from diffusion constraints [5, 6].

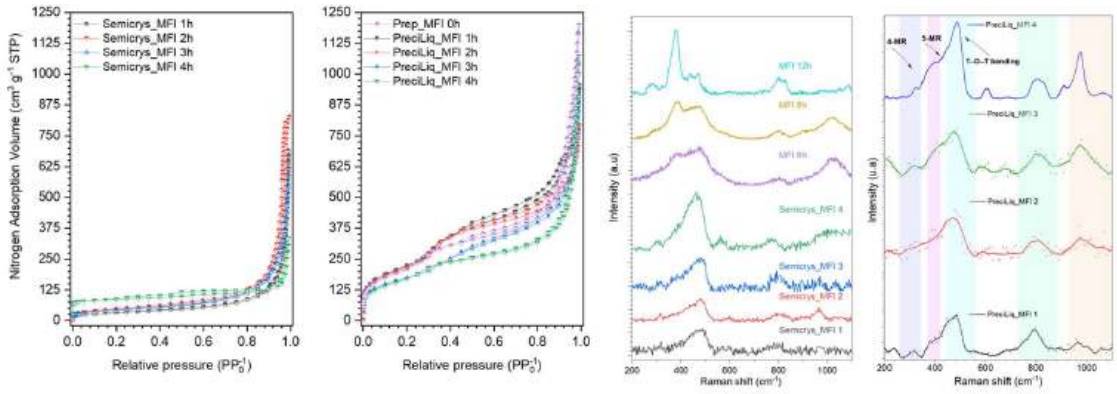

Figure 1. (left) Isotherms of nitrogen adsorption at 77 K over the partial crystalline solids and the precipitates from MFI gels. UV-Raman spectra of the partial crystalline solids and the precipites of (right) MFI.

The present study demonstrates how partial crystallization pathways and solution-mediated chemistry can be harnessed as chemical design principles to catalyze new reactions by controlling local structure, disorder, and reactivity beyond conventional crystalline limits.

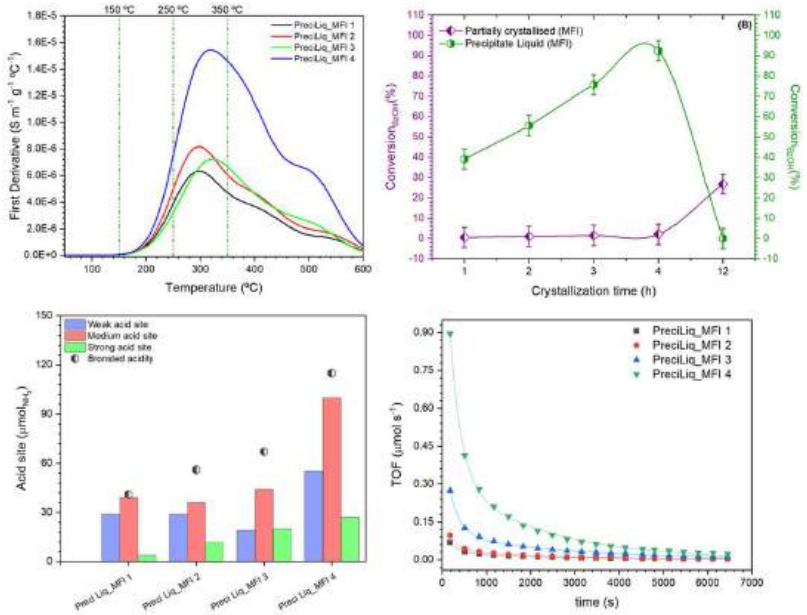

Figure 2. (Left)Acidity of precipitated materials. Conversion for the Friedel-Crafts alkylation of benzyl alcohol with o-xylene (right top), and TOF cracking of 1,3,5-triisopropylbenzene (TIPB) (right bottom).

Acknowledgment: This study forms part of the Advanced Materials programme and was supported by MCIN with funding from European Union NextGenerationEU (PRTR-C17.I1) and by Generalitat Valenciana.

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CCS - D2 - O17

Tailoring vanadium-impregnated small-pore zeolite(CHA) catalysts: Effects of synthesis on structure and non-oxidative and CO_2-assisted propane dehydrogenation performance

Iqtidar Ali Khan[1], Jose A. Mendoza Mesa[1], Max Bols[2], Run Zou[1], Michiel Dusselier[1]
[1]KU Leuven, Belgium; [2]University of Ghent, Belgium

Propene is a key petrochemical feedstock traditionally produced as a byproduct of oil-based cracking processes, such as fluid catalytic cracking (FCC) and steam cracking (SC), which are energy intensive and associated with significant CO_2 emissions. Non-oxidative propane dehydrogenation (PDH) is the primary commercial on-purpose route to propene, but it relies on Cr(toxic) and Pt (expensive) catalysts that suffer from rapid deactivation due to coke formation and sintering, leading to frequent regeneration and increased environmental and economic costs.

To address these challenges, utilizing CO_2 as a soft oxidant for propane dehydrogenation (OPDH) suppresses coke formation, enhances propene yields, and coproduces CO, yet another platform chemical. Initial studies in our laboratory identified V-based catalysts as highly effective for OPDH[1]. Notably, vanadium species confined in small-pore zeolites[2] exhibit comparable activity to those on mesoporous supports despite lower vanadium loadings when normalized by apparent surface density[3].

In this work, we investigate VO_x-supported chabazite (CHA) catalysts for non-oxidative PDH and CO_2-assisted OPDH. CHA-40 (Si/Al ≈ 30, ICP) was synthesized via interzeolite conversion (IZC) from USY zeolite (CBV780). Vanadium was incorporated using incipient wetness impregnation (IWI) and wet impregnation (WI), targeting an optimized loading of 1.3 mmol $V \cdot g_{support}^{-1}$. Key synthesis parameters includes sonication time during precursor solution preparation and the ammonium metavanadate to oxalic acid ratio.

Catalytic performance was evaluated using box-whisker plots (Fig. ***2***a) that integrate time on stream behavior with space-time yield, providing a comprehensive visualization of catalyst stability and activity. Longer sonication times and the use of WI led to lower OPDH activity. Corresponding H_2-TPR results (Fig. ***2***b) indicate increased formation of polymerized VO_x species reducible at higher temperatures under these conditions. Complementary PXRD and UV-Vis DR analyses confirm a clear synthesis-structure-activity relationship. These results demonstrate that tailored VO_x/CHA catalysts provide a sustainable, Cr- and Pt-free route for efficient propane dehydrogenation and CO_2 utilization.

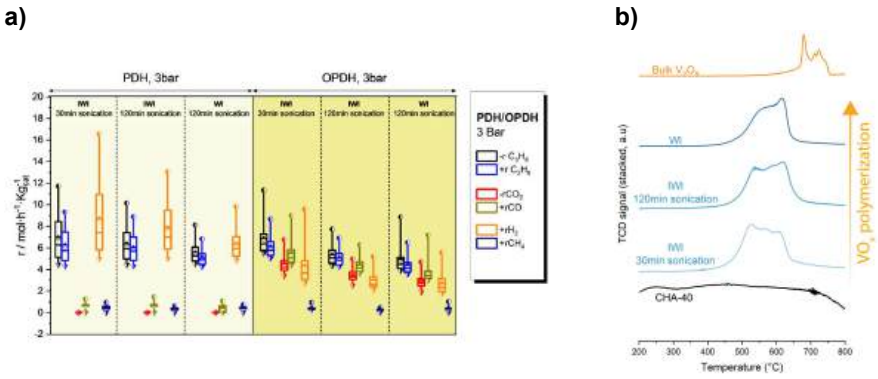

Fig. 2. (a) Box-whisker plots of reactant consumption ($-rC_3H_8$, $-rCO_2$) and product formation ($+rC_3H_6$, $+rCO$, $+rH_2$, $+rCH_4$) at 3 bar PDH and OPDH for 1.3V/CHA-40 catalysts prepared under different synthesis conditions. Reaction conditions: 200.0(2)mg 125-250µm catalyst,600°C,1bar $CO_2/C_3H_8/Ar/N_2$ of 2.5/2.5/10/85 $Nml \cdot min^{-1}$,WHSV 1.5g C_3H_8 $gcat^{-1}h^{-1}$ **(b)** H_2-TPR profiles of catalysts at constant V loading of 1.3 $mmolV \cdot g^{-1}$ and NH_4VO_3: Oxalic acid ratio of 1:2 using different impregnation strategies(IWI with 30 and 120min sonication and WI)

Acknowledgements: Project funded by the Moonshot cluster SBO D2M2 (HBC.2022.0538).

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CCS - D2 - O18
Sustainable copper(I) catalysts for CuAAC: Mechanochemistry, structure and mechanism

M.S. Viana[1], R. Rodrigues[1], B.P. Machado[1], M. Outis[1], N.A.G. Bandeira[2], V. Rosa[1], C.S.B. Gomes[1]
[1]*LAQV-REQUIMTE, NOVA School of Science and Technology, NOVA University of Lisbon, Portugal*
[2] *BioISI, Faculdade de Ciências da Universidade de Lisboa, Portugal*

The copper-catalysed azide–alkyne cycloaddition (CuAAC) is a well-known "click" reaction that is highly regarded for its robustness, efficiency, and broad range of applications. Despite its maturity, the development of highly active, sustainable and well-defined copper(I) catalytic systems remains an active area of research.[1,2] Building on our previous report on the efficient operation of cationic heteroleptic aryl-BIAN copper(I) complexes under neat conditions at room temperature,[3] we expand this catalyst family and explore mechanochemistry as a greener synthetic alternative.
In this study, we present the synthesis of a series of novel cationic heteroleptic copper(I) complexes, which were prepared using both solution-based and mechanochemical methodologies. Notably, mechanochemistry enabled access to specific complexes that could not be obtained through conventional solution-based methods. Selected copper(I) species, including [Cu(BIAN)(PPh_3)(ONO_2)] and [Cu(BIAN)(PPh_3)$_2$]NO_3, were isolated and fully characterised using spectroscopic methods and single-crystal X-ray diffraction. This provided detailed structural insights into ligand coordination and nitrate binding modes.
Density functional theory (DFT) calculations were employed to rationalise the experimental observations and elucidate the mechanistic pathway governing interconversion between distinct copper(I) species. These calculations reveal the thermodynamic preference for the ionic nitrate complex and identify the key intermediate and transition states associated with Cu–O bond formation and cleavage. Overall, this work highlights the synergy between mechanochemistry, crystallography, and computational chemistry in developing efficient and sustainable CuAAC catalysts, while offering new insights into their structural dynamics and reaction mechanisms.

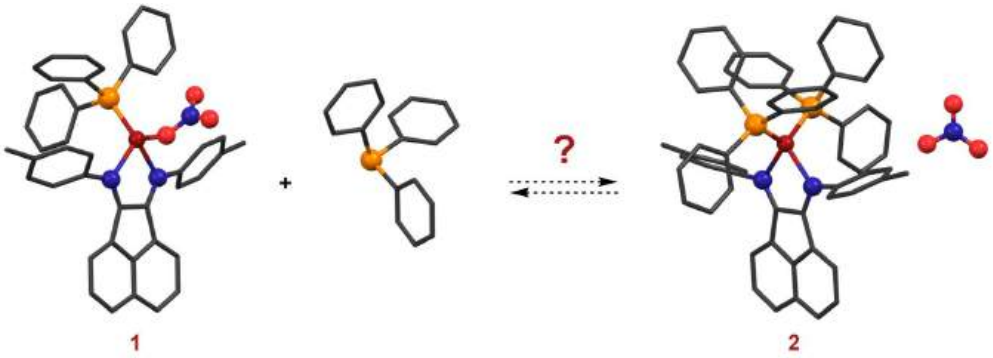

Fig. 1. Equilibrium between the two copper(I) complexes.

This work was supported by FCT/MCTES through projects UID/50006/2025, UID/PRR/50006/2025 and LA/P/0008/2020 of the Associated Laboratory for Green Chemistry - LAQV REQUIMTE (https://doi.org/10.54499/UID/50006/2025, https://doi.org/10.54499/UID/PRR/50006/2025 and https://doi.org/10.54499/LA/P/0008/2020 and contract 2023.11076.TENURE.117, and by EU funded project IMPACTIVE (no. 101057286).

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CCS - D2 - F01
Nanopatterned chemically modified carbon surfaces for carbohydrate valorization

Maarten Mulier[1,2], Kunal S. Mali[1], Sophie Hermans[2], Steven De Feyter[1]
[1]Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Belgium; [2]Institute of Condensed Matter and Nanosciences (IMCN), MOST Division, UCLouvain, Belgium

As interest in sustainable, greener and more efficient chemical processes grows, carbon materials are emerging as an attractive alternative to traditional catalysts. In this project, we are designing mono- and multifunctional carbocatalysts for the conversion of cellulose from lignocellulosic biomass into valuable chemical compounds. In proof-of-concept experiments, catalytically active functional groups will be attached to well-defined and model carbon surfaces, such as highly oriented pyrolytic graphite (HOPG). This approach allows for detailed nanoscale characterization of the modified surface. Once established, these functionalization strategies can be extended to real-world, well-defined and practical carbon materials, including graphite and graphene powders, that can be used for catalysis, but where precise characterization is more difficult.
The design of the carbocatalysts is made possible via the introduction of active sites through controlled surface functionalization with radical diazotization. Advanced characterization techniques such as Raman spectroscopy, AFM, and STM will be employed to gain initial insights into the structure and spatial arrangement of active sites on model carbon surfaces. TGA-MS, XPS, CHNS, UV-Vis and Boehm titration will be leveraged for the characterization of real-world carbon materials.
The mono- and multifunctional carbocatalysts can be tailored through spatial control of active sites achieved by concentration regulation, or the application of self-assembled monolayers as masks. This approach permits to fine-tune the reaction pathways and investigate how the spatial control of active sites influences catalytic performance. Combining KU Leuven's surface engineering expertise with UCLouvain's knowledge in catalysis, our goal is to design efficient, selective, and reusable catalysts that enable cleaner, more sustainable production of bio-based fine chemicals.

Acknowledgements: Financial support from the Research Foundation-Flanders and KU Leuven–Internal Funds (C14/23/090) is acknowledged, as well as KU Leuven Global PhD Partnerships with UCL (GPUCL/24/021).

CCS - D2 - F02

Spin frustration and its role in stability and reactivity of first-row transition metal MOFs

Patrick Lechner[1,2], Fuli Sun[1], Gaurab Ganguly[1], Michael J. Sahre[3], Georg Kresse[3,4], Johannes C. B. Dietschreit[1], Leticia González[1]*

[1]Institute of Theoretical Chemistry, University of Vienna, Austria; [2]University of Vienna, Vienna Doctoral School in Chemistry, Austria; [3]University of Vienna, Faculty of Physics, Austria; [4]VASP Software GmbH, Austria

Iron-based MOFs with a triangular metal center—particularly MIL-88B, MIL-100, and MIL-101—have emerged as exceptional catalysts, demonstrating a remarkable ability to catalyze N_2 fixation.[1] The electronic structure of the triangular nodes is often approximated by a ferromagnetic arrangement. Recently we demonstrated spin frustration as a defining feature of these nodes—arising from competing α- and β-spin alignments of the Fe^{3+} centers—that shapes both structure and reactivity.[2] Using spin-flip, broken-symmetry DFT, we modeled a spin-frustrated antiferromagnetic ground state that allowed us to explain the MOFs temperature-dependent chemistry: at ambient conditions, it enhances N_2 fixation, while its partial loss upon heating favors CO adsorption through π-backbonding. By systematically scanning the library of first-row metals (M = Ti, V, Cr, Mn, Fe, Co), we uncover distinct trends in the degree of spin frustration in the ground state and in N_2 binding strength. This trend demonstrates that Fe^{3+} is an exceptional case. This work highlights spin frustration as an intrinsic electronic feature of triangular $M_3(\mu_3\text{-O})$ nodes, providing a new perspective on how correlated spin states can modulate reactivity and small-molecule binding in metal–organic frameworks.

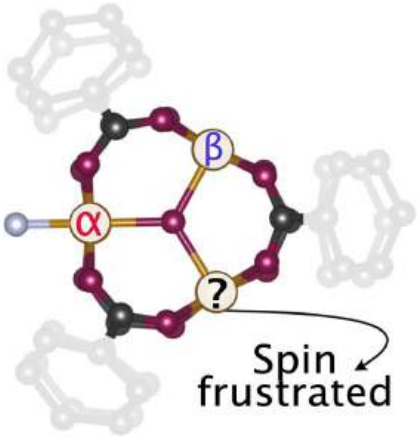

Fig. 1. The frustrated spin on the third metal atom, indicated by a question mark, must choose between α- and β-spin alignment, resulting in the phenomenon known as spin frustration.

This study is funded by the Austrian Science Fund (FWF) within the Cluster of Excellence “Materials for Energy Conversion and Storage” [grant 10.55776/COE5].

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CCS - D2 - F04

Covalent functionalization of carbon surfaces with phenyl sulfonic acid for nanostructured, bifunctional catalysts in biomass chemical transformations

Jean Cedric Madrigalejo[1], Steven De Feyter[1]
[1]*Division of Molecular Imaging and Photonics, Dept. of Chemistry, KU Leuven, Belgium*

Heterogeneous catalysts based on carbon (e.g. graphene) can be engineered as novel bifunctional catalysts—with both covalent and non-covalent active sites[1,2]—for cooperative performance in relevant biomass transformations while maintaining stability and recyclability. We focus on the covalent functionalization of phenyl sulfonic acid ($–SO_3H$) species on carbon surfaces using diazonium chemistry. First, highly oriented pyrolytic graphite (HOPG) serves as a model surface to optimize grafting, then the protocol is translated to bulk graphene flakes for the nano-patterned grafting of the Brønsted acid sites enabling precise control over loading and spatial distribution.

A comprehensive suite of characterization techniques is used for understanding the catalyst structure in the microscopic and bulk level. The catalyst's morphology (layer thickness, roughness, and flake size) is described using atomic force microscopy (AFM), together with scanning tunneling microscopy (STM) imaging of the nano-structured arrangement of grafted species. Quantification of the degree of functionalization is done through Raman spectroscopy and mapping, elemental analysis, X-ray photoelectron spectroscopy (XPS), and thermogravimetric analysis (TGA).

Eventually, bifunctionality will be incorporated to the carbon through a non-covalently attached catalytic moiety (via pyrene-based π–π adsorption) with translational mobility on the carbon surface, which promises cooperative and adaptive performance in catalyzing valuable biomass transformation reactions.

Acknowledgement: We acknowledge support from KU Leuven (C1 C14/23/090), and iBOF program BOF/25/022.

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CCS - D2 - F05

Beyond catalyst immobilization: Engineering local proton donor microenvironments for CO_2 electroreduction

Milda Tomy[1], Kunal S Mali[1], Marc Robert[2], Steven De Feyter[1]
[1]Division of Molecular Imaging and Photonics, Dept. of Chemistry, KU Leuven, Belgium; [2]Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire, France and Institut Universitaire de France, France

One of the most important steps toward energy storage and sustainability is the conversion of CO_2 into value-added products. Catalysts with high activity, selectivity, and durability are needed to achieve this effectively. Heterogeneous molecular catalysts (HMCs) offer a unique solution to it by combining the robustness and recyclability of the heterogeneous catalysts with the molecular precision and tunability of the homogeneous ones. This is achieved by immobilizing well-defined molecular catalysts on conductive supports, thereby offering excellent control over catalytic structure and reactivity.

We present a design concept in this work that extends beyond conventional catalyst immobilization. 2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphine iron(III) chloride is self-assembled on highly oriented pyrolytic graphite (HOPG) that has been functionalized by covalently grafted benzene carboxylic acid groups. These surface-bound carboxylic acid moieties act as proximal proton donors, mimicking key features of enzymatic active sites. This architecture enables systematic investigation of how proton accessibility and spatial organization influence CO_2 reduction performance.

Local proton donors placed close to the catalytic centers provide key insight into how local proton availability influences the catalysis and guides the design of more efficient heterogeneous molecular catalysts. Thus, this work lays a framework for investigating the fundamentals of CO_2 electroreduction while precisely controlling the active sites and their surrounding chemical environment.

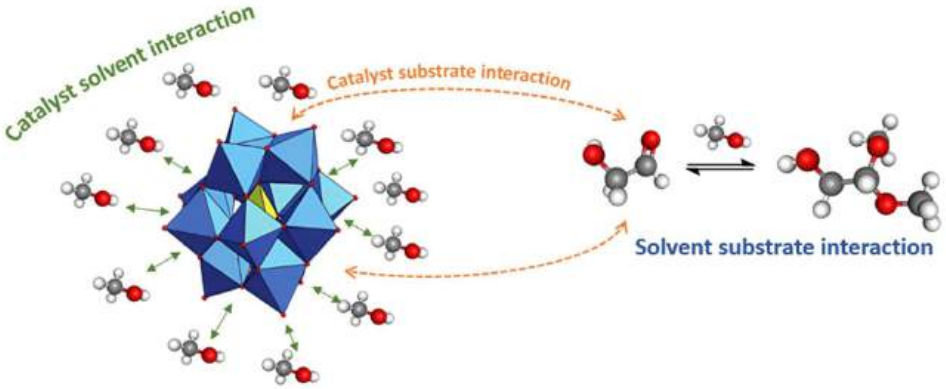
Acknowledgements: Financial support from the Research Foundation-Flanders (FWO G0A5U24N) and KU Leuven–Internal Funds (C1 C14/23/090) is acknowledged.

CCS - D2 - F07

Theoretical and experimental investigations of acetal formation during the oxidation of xylose to formic acid catalysed by $H_5PV_2Mo_{10}O_{40}$ in methanolic-aqueous solution

Leon Schidowski[1], Alexander Buck[1], Maximilian J. Poller[1], David Robinson[2], Jakob Albert[1]*
[1]Institute of Technical and Macromolecular Chemistry, Universität Hamburg, Germany; [2]Dept. of Chemistry and Forensics, Nottingham Trent University, UK

Biomass, including carbohydrates, lipids and lignocellulose is an attractive alternative feedstock for the chemical industry as it is the only available regenerative carbon source on earth. Therefore, catalytic biomass valorisation is gaining both scientific and industrial interest. One promising process is the Erlanger OxFA process that aims for the bio-based production of formic acid using a Keggin-type polyoxometalate catalyst [1] It has been found that by using methanol as a (co-)solvent, Keggin-type POM catalysts can completely suppress undesired total oxidation to CO_2 under oxidative conditions. This drastically enhances the carbon efficiency from biomass compared to the state-of-the-art technologies to close to 100% yield in formic acid (FA) methyl ester [2]. In this study, we aimed for answering the fundamental research question what are the key mechanisms in aqueous-alcoholic solutions preventing decarboxylation and where are the limits with respect to process conditions and solvent composition.



Therefore, a special focus was on the influence of the functional groups in different reaction intermediates from HPA-2 ($H_5PV_2Mo10O40$) catalyzed xylose oxidation on the way to formic acid. Moreover, we found out that the protection of reactive functional groups of the model carbohydrates is depending on the formation and stability of several reaction intermediates via acetalization or esterification. This is strongly dependent on solvent composition and reaction conditions. The present findings were supported by DFT-calculations explaining the different effects the solvent composition exhibits on both substrate and catalyst, emphasizing the catalyst-solvent interactions as the superior ones for catalysis.

Keywords: Polyoxometalate, biomass valorisation, OxFA process, solvent effects, DFT calculations

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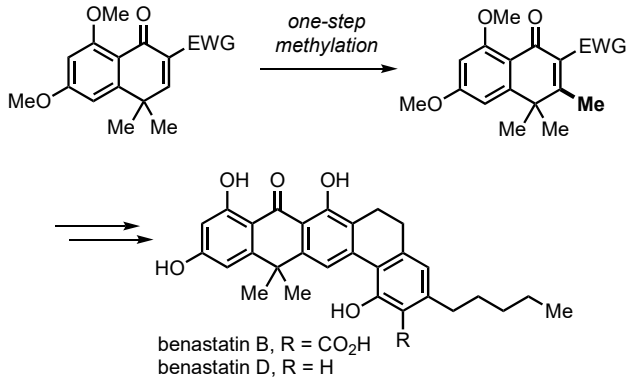
CCS - D3 - O02
Direct β-methylation of α-activated cycloalkenones: Total synthesis of benastatins B and D

Chien-Chung Lee[1], Kak-Shan Shia[2], Yen-Ku Wu[1]
[1]National Yang Ming Chiao Tung University, Taiwan; [2]National Health Research Institutes, Taiwan

We have developed a transition metal-free, direct β-methylation of cycloalkenones (Scheme 1). This transformation proceeds via cycloaddition between trimethylsilyldiazomethane and the activated alkene, followed by rearrangement of the resulting adduct to deliver β-methylated products. The method is general and efficient, furnishing over 30 examples in up to 93% yield. Mechanistic studies, including deuterium-labeling experiments, are consistent with a 1,2-hydrogen shift pathway in the rearrangement. Application of this formal C–H methylation in combination with our previously reported anionic annulation strategy[1] enabled total syntheses of natural antibiotic benastatin B[2] and benastatin D.[3]



Scheme 1. A synthetic approach to benastatins B and D.

We acknowledge the financial support to this work by the National Science and Technology Council of Taiwan.

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CCS - D3 - O03
New strategies for sustainable base catalysis through metal cluster design

Belén Lerma-Berlanga[1], Lluís Martínez Belenguer[1], Yongkun Zheng[1] and Antonio Leyva-Pérez[1,*]
[1]Instituto de Tecnología Química. Universitat Politècnica de València–Agencia Estatal Consejo Superior de Investigaciones Científicas, Valencia, Spain

Transesterification and related base-catalyzed nucleophilic alcohol addition reactions are key transformations in sustainable chemistry, underpinning the production of biodiesel and high-value organic carbonates such as ethyl methyl carbonate (EMC), relevant in lithium-ion batteries and fuels. Here, we demonstrate the versatility of inorganic metal-based nanoclusters as catalytic platforms, highlighting the role of confinement, nanoscale organization, and chemical environment.
First, we present zeolite-confined alkaline oxide nanoclusters for selective EMC synthesis.[1] Commercial NaX already shows significant catalytic activity, achieving EMC with high selectivity and reusability over ten cycles, including continuous-flow operation. Incorporation of alkaline and alkaline-earth salts and oxide clusters, particularly K_2O and MgO, enhances performance, reaching yields up to 99% without reactive distillation while maintaining selectivity (up to 65%). This approach is effective for NaX, NaY, H-USY, H-ZSM-5, and H-BETA, which otherwise show limited activity. In parallel, we investigate sustainable, ligand-free sub-nanometric $MgCO_3$ clusters organized as gel-like systems, synthesized via CO_2 sequestration in bioavailable ethanol.[2] These nanoclusters are four times more active than calcium analogues in dimethyl carbonate transesterification and display turnover frequencies up to 40 times higher than bulk $MgCO_3$. Their enhanced performance arises from the hard Lewis acidic nature of Mg^{2+}, stabilized yet highly accessible within the nanostructured carbonate network.

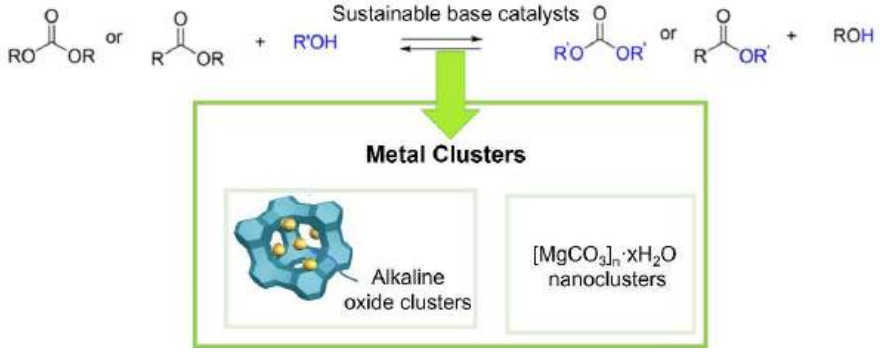

Fig. 1. Two complementary strategies for base-catalyzed alcohol transformations: (A) Zeolite-confined alkaline/alkaline-earth oxide nanoclusters. (B) Gel-like ligand-free $MgCO_3$ sub-nanometric clusters.

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CCS - D3 - O04

Superior efficacy of selenium-promoted cobalt titanate in dual catalysis: Bisindole synthesis and acetophenone hydrogenation

Boopathi Shagunthala Hariprasad, Sundaram Ganesh Babu*
Nano-Catalysis Research Lab, Dept. of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, India

Non-metal-promoted metal titanates are synthesized *via* a novel surface-loading approach, wherein controlled weight percentages of non-metals (C, P, S, or Se) are deposited onto pre-formed cobalt titanate ($CoTiO_3$), followed by calcination at their respective melting temperatures.[1] This method aims to investigate the promotional role of surface-loaded non-metals in modulating the catalytic behaviour of $CoTiO_3$ toward bisindole synthesis and transfer hydrogenation of acetophenones. The catalytic performance exhibits the following trend: Se–$CoTiO_3$ ≈ S–$CoTiO_3$ > C–$CoTiO_3$ > P–$CoTiO_3$, which directly correlates with the surface charge characteristics and electron-donating ability of the promoters.[2] Among the series, selenium- and sulfur-promoted $CoTiO_3$ showcase notably enhanced activity during optimization, attributed to improved surface basicity and charge transfer interactions. However, the S–$CoTiO_3$ catalyst demonstrates poor stability with a marked decline in yield upon recycling, likely due to surface site poisoning and active phase deactivation. In contrast, Se–$CoTiO_3$ retains outstanding catalytic activity and durability over seven consecutive reaction cycles, underscoring the superior reusability and structural stability. The analytical techniques confirm the stable incorporation of selenium into the surface lattice, evidencing the robustness and resistance to leaching under reaction conditions. Overall, the selenium-promoted $CoTiO_3$ catalyst exhibits an optimal balance between surface charge modulation and structural integrity, identifying selenium as a sustainable non-metal promoter for enhancing titanate-based catalytic systems. From fig.1, the study provides valuable insights into rational surface engineering strategies for improving the efficiency and stability of heterogeneous catalysts in green organic transformations.

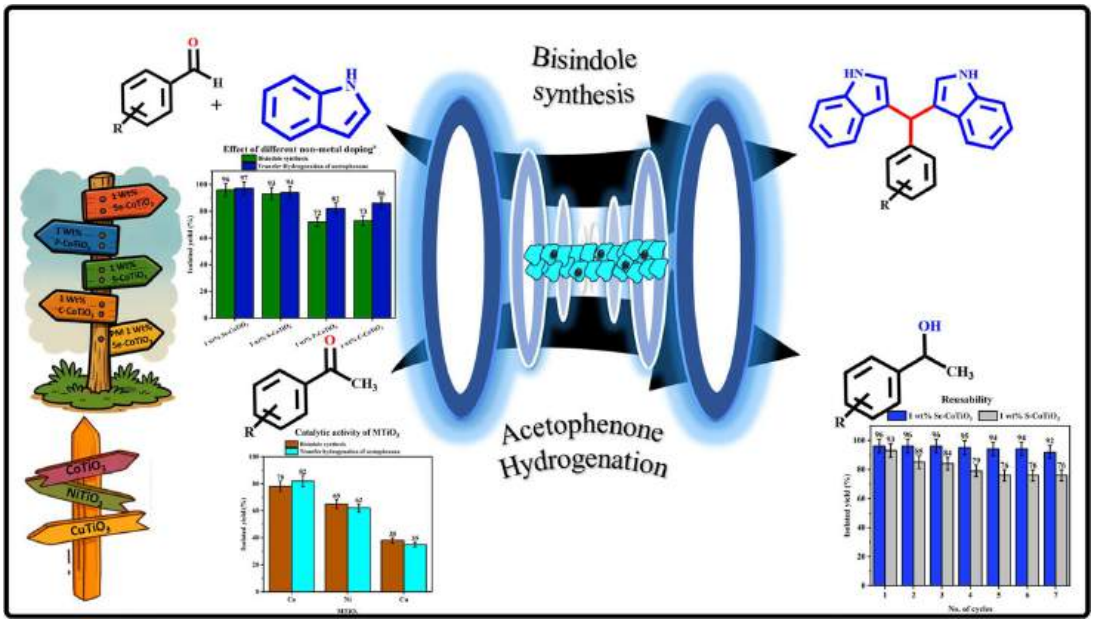

Fig. 1. Overview of non-metal-promoted cobalt titanate in dual catalysis.

This work was financially supported by Vellore Institute of Technology (VIT), Vellore, under the Faculty Seed Grant (RGEMS) (sanction Order No.: SG20250058), VIT management for characterization support, and infrastructure. BSH acknowledges VIT for providing the fellowship.

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CCS - D3 - O05

Synthesis of axially chiral P,N ligands exploiting non-covalent bonding interactions and their application in asymmetric catalysis

Sarah Smoni Varghese,Patrick J. Guiry*
University College Dublin, Ireland

The synthesis and application of UCD-Phim, a P,N ligand containing both central and axial chirality, was reported by the Guiry group in 2017.[1] In UCD-Phim, π-π stacking interactions was observed between the electron-deficient pentafluorobenzyl group and the electron-rich naphthalene group. This interaction provides configurational stability around the chiral axis, however the ligand starts to epimerise at temperatures greater than 40 °C, which limits its application in high temperature catalysis. In this project the electronics around the ligand backbone was varied in order to improve π-π stacking interactions between the two aryl systems. A library of novel axially chiral P,N ligands have been synthesised, and the ligands with a heptafluoronaphthalene moiety, has shown to have higher π-π stacking interactions due to the increased electron-deficient character of the aryl ring. The barrier to rotation of the novel ligands have been investigated using VT-NMR spectroscopic techniques and calculated to be 27.5 kcal/mol which is higher than that previously reported for UCD-Phim (Fig. 1).

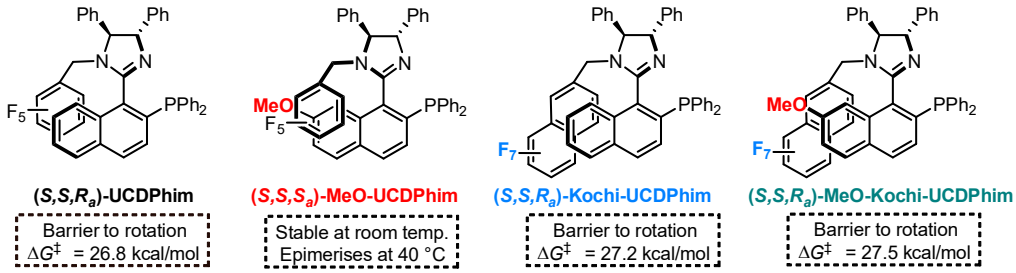

Fig. 1. Synthesised axially chiral P,N ligands and a comparison of their barrier to rotation

Phthalazine and dihydrophthalazine derivatives are prevalent in pharmaceutical compounds.[2] 1-Alkynyl-1,2-dihydrophthalazines can be accessed enantioselectivity *via* copper-catalysed alkynylation of phthalazinium salts. This expands on the work done by Chen and co-workers, where the racemic alkynylation scope was explored.[3] Optimisation of the copper-catalysed alkynylation on the model substrate is described, obtaining the alkynylated product in high yields and enantioselectivities (Fig. 2), future work will involve the expansion of the substrate scope.

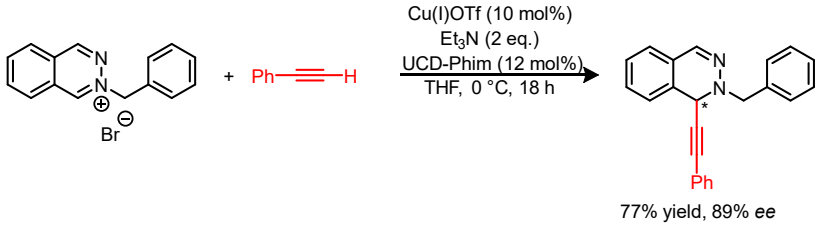

Fig. 2. Enantioselective alkynylation of phthalazinium salts

[1]Rokade, B. V.; Guiry, P. J. *ACS Catal.* **2017**, 7 (4), 2334-2338.
[2]Velázquez, M.; Fernández, R.; Lassaletta, J.; Monge, D. *Org. Lett.* **2023**, *25* (49), 8797-8802.
[3]Gao, G.; Luo, M.; Guo, F.; Liang, K.; Zhou, F.; Chen, Q. *Adv. Syn. Cat.* **2020**, 362 (12), 2332–2336.

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CCS - D3 - O06
Beyond mixing: Quad-screw extruder as a chemical reactor for solvent-free organic synthesis

Paolo Freisa[1], Alessandro Barge[1], Giancarlo Cravotto[1]
[1]Dept. of Drug Science and Technology, University of Turin, Italy

Extrusion is a well-established continuous processing technology employed in several industrial sectors, particularly in polymer manufacturing[1] and in the food sector[2]. In recent years, extrusion has attracted increasing interest in organic chemistry and pharmaceutical research, as it enables the direct use of mechanical energy (shear, compression and friction) to drive chemical reactions under solvent-free conditions. In this context, reactive extrusion allows the extruder to operate as a real chemical reactor, in line with the principles of process intensification and green chemistry[3,4]. In this study, we investigate the potential of a quad-screw extruder (Technovel, Osaka, Japan) equipped with four modular screws featuring conveying, reverse and kneading elements, two independent feeders and six independently controlled heating zones. This configuration provides flexibility and precise control of residence time, temperature and mechanical stress. We demonstrate the possibility of conducting three different classes of organic reactions under solvent-free conditions. First, a condensation reaction between vanillin and dimedone was successfully performed, affording an acridine-1,8-dione substructure. Subsequently, direct amidation reactions between carboxylic acids and amines were achieved extruding the corresponding ammonium salt. Finally, the capability of the extruder to promote pericyclic reactions was demonstrated, exploiting its ability to operate at elevated and well-controlled temperatures. All reactions were carried out in continuous mode, drastically reducing reaction times and eliminating the need of solvents and activating agents and highlighting the crucial role of enhanced thermal transfer and intense mechanical activation. Overall, this work showcases quad-screw reactive extrusion as a sustainable and industrially relevant platform for organic synthesis.

[1]Hyvärinen, M.; Jabeen, R.; Kärki, T. *Polymers* **2020**, 12, 1306.
[2]Yi, C.; Qiang, N.; Zhu, H.; Xiao, Q.; Li, Z. *Food Research International* **2022**, 160, 111681.
[3]Freisa, P.; Lattuada, L.; Barge, A.; Cravotto, G. *RSC Mechanochemistry* **2026**.
[4]Crawford, D. E. *Beilstein Journal of Organic Chemistry* **2017**, 13, 65-75.

CCS - D3 - O07

From support to catalyst: Redefining the role of the carbon in thermochemical hydrogenation reactions

Jakub Kusz[1], Markus Antonietti[1], Mateusz Odziomek[1]
[1]*Colloid Chemistry Dept., Max Planck Institute of Colloids and Interfaces, Germany*

Typical hydrogenation catalysts consist of noble metal nanoparticles, such as Pt nanoparticles (PtNPs), dispersed on porous carbon supports. In such systems, catalytic activity is generally attributed almost exclusively to the metal phase. However, recent studies have shown that properly engineered carbon materials (noble carbons) can themselves act as efficient metal-free catalysts. At the same time, thermochemical hydrogenations are commonly described by the Langmuir–Hinshelwood mechanism, in which molecular hydrogen dissociates on an active site and subsequently reacts with an adsorbed organic substrate. The possibility that the carbon support actively participates in hydrogenation, therefore challenges this traditional view.

By employing the reduction of *p*-nitrophenol to *p*-aminophenol as a model reaction, we demonstrate that the carbon support in PtNPs-based catalysts plays an active catalytic role. While PtNPs are required for the initial hydrogen activation, the subsequent reduction of the nitro group occurs efficiently on the carbon support, independently of PtNPs. The kinetics of this step can be tuned by controlling the carbon's properties, such as morphology and heteroatom doping. Using TCNQ-derived noble carbon, we demonstrate that tuning the support can lead to activities exceeding those of the PtNPs. Moreover, electrochemical studies further reveal that two carbon catalysts put in contact may influence mutually their potential, leading to synergistic effects. These findings represent a significant advance in the development of noble carbons and provide new mechanistic insight into support-catalyst synergy, highlighting their potential as viable alternatives to noble-metal-based hydrogenation catalysts.

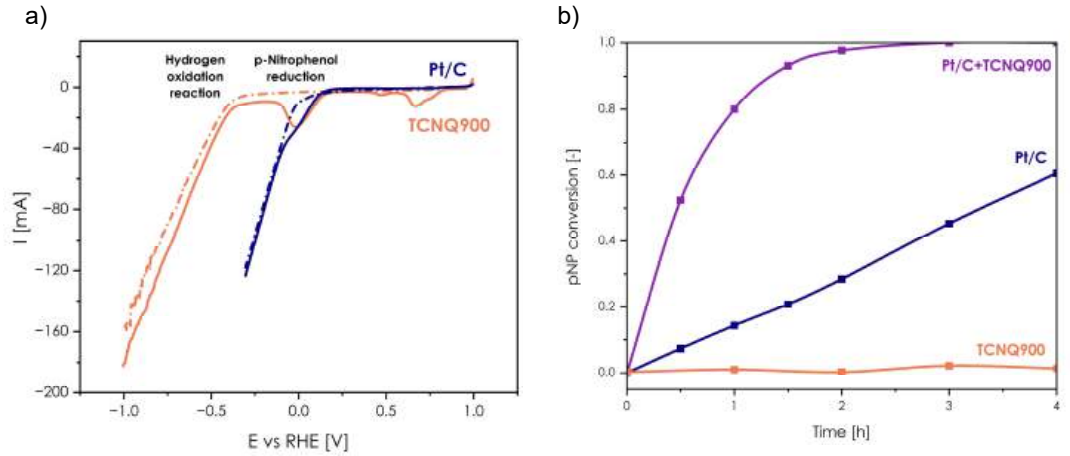

Figure 1. (a) Electrochemical study of hydrogen oxidation and p-nitrophenol reduction on Pt/C and TCNQ900 carbons, and (b) p-nitrophenol thermochemical reduction enabled through synergistic effect between the two carbon catalysts.

[1]Antonietti, M.; Oschatz, M. *Adv*. Mater. **2018**, *30(21),* 1706836.
[2]An, H., et al. *ACS Catalysis* **2022**, *12(24)*, 15021-15027.
[3]Dinakar, B., et al. *J. Am. Chem. Soc*. **2025**, *147(51)*, 46752-46758.

CCS - D3 - O08
Unlocking nonalternating ethylene–CO copolymerization via ligand-controlled isomerization

Michele Tomasini[1], Yajun Zhao,[2] Stefan Mecking[2], Lucia Caporaso[1]
[1]Dept. of Chemistry, University of Salerno, Italy; [2]Dept. of Chemistry, University of Konstanz, Germany

Nonalternating ethylene–carbon monoxide copolymerization remains a fundamental challenge due to the strong preference of CO for coordination and insertion at late transition-metal centers, which promotes alternating sequences and catalyst deactivation (Figure 1a). Previous studies have shown that productive chain growth critically depends on the ability of the catalyst to undergo cis/trans isomerization of chelated Ni(II) intermediates, a prerequisite for consecutive ethylene insertions.[1]
Phosphine–phenolate Ni(II) catalysts reported in the literature represent a benchmark system for accessing nonalternating microstructures.[2,3] Computational studies have demonstrated that, in these systems, isomerization proceeds through high-energy transition states that are only weakly stabilized by η² interactions between aryl substituents and the nickel center, thereby limiting catalytic activity and CO tolerance.
In this work, we introduce a new class of neutral Ni(II) catalysts with enhanced CO tolerance and superior CO incorporation properties. DFT calculations reveal that polymerization proceeds through a sequence of coordination, isomerization, and insertion steps, with cis/trans isomerization emerging as a key mechanistic bottleneck. Crucially, the presence of P-bound oxygen-containing aryl substituents enables intramolecular Ni–O interactions that stabilize square-pyramidal transition-state geometries during isomerization (Figure 1b). This interaction significantly lowers the isomerization barriers compared to Ni–aryl-stabilized analogues, thereby facilitating rapid access to productive ethylene insertion pathways and suppressing deactivation pathways.[4] Overall, this study highlights cis/trans isomerization as the central selectivity-determining step and demonstrates how targeted modulation of metal–ligand interactions can be exploited to control polymerization pathways at the molecular level.

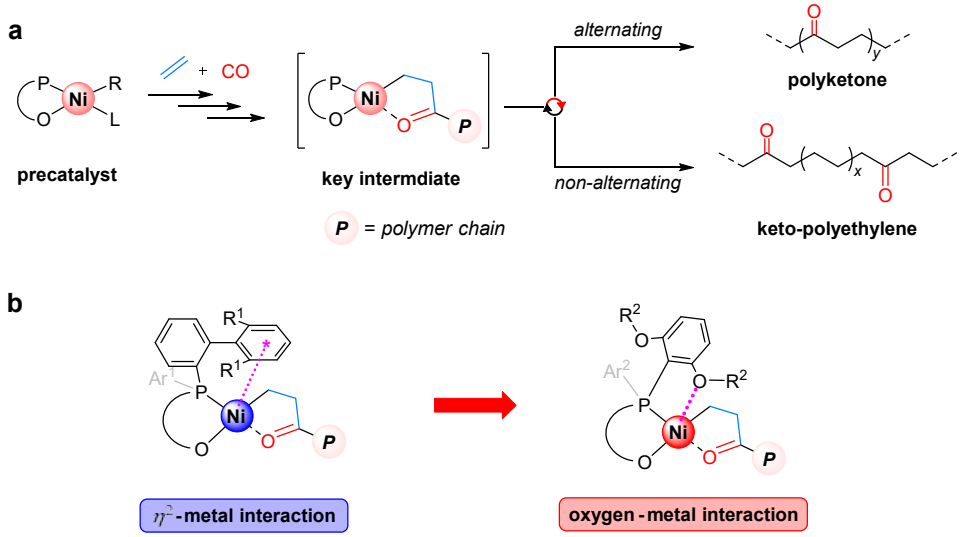

Fig. 2. a. Proposed mechanism of ethylene-CO copolymerization mediated by key intermediate. **b.** Noncovalent interactions in varying catalyst systems

[1]Haras, A.; Michalak, A.; Rieger, B.; Ziegler, T. *J. Am. Chem. Soc.* **2005**, *127*, 8765.
[2]Baur, M.; Lin, F.; Morgen, T. O.; et al. *Science* **2021**, *374*, 604.
[3]Voccia, M.; Odenwald, L.; Baur, M.; et al. *J. Am. Chem. Soc.* **2022**, *144*, 15111.
[4]Odenwald, L.; Wursthorn, L.; Mecking, S. *J. Am. Chem. Soc.* **2025**, *147*, 7182.

CCS - D3 - O09

Structure–reactivity relationships in imidazopyridine complexes of Mo(VI), W(VI) and V(IV) for olefin epoxidation catalysis

Vera Barrutia Fernando A.[1], Amézquita Valencia Manuel[1*]
[1]*Dept. of Inorganic Chemistry, Instituto de Química, Universidad Nacional Autónoma de México, México*
**Email: manuel.amezquita@iquimica.unam.mx*

Olefin epoxidation is a transformation of major relevance in chemical industry, as epoxides are key intermediates in the production of polymers, fine chemicals, pharmaceuticals, and advanced materials. Conventional epoxidation methods often rely on stoichiometric oxidants such as peroxides, permanganates, or dichromates, which pose environmental and safety concerns due to toxicity and the generation of hazardous byproducts. Consequently, the development of efficient and selective catalytic systems operating under mild conditions remains highly desirable.

In this work, a family of molybdenum(VI) complexes featuring a cis-$[MoO_2]^{2+}$ core coordinated to imidazopyridine-based ligands was synthesized and evaluated as catalysts for olefin epoxidation. The catalytic performance of these complexes was systematically investigated through optimization of key reaction parameters, including solvent, oxidant, catalyst loading, and reaction time, in order to identify the most efficient catalytic system in terms of conversion and selectivity.

Building on these results, structurally analogous vanadium(IV) and tungsten(VI) complexes bearing $[VO]^{2+}$ and cis-$[WO_2]^{2+}$ cores, respectively, and coordinated to the same imidazopyridine ligand framework, were synthesized and evaluated under the optimized conditions established for the molybdenum catalysts. Comparative studies revealed that the nature of the metal center and the ligand environment play a critical role in determining catalytic activity.

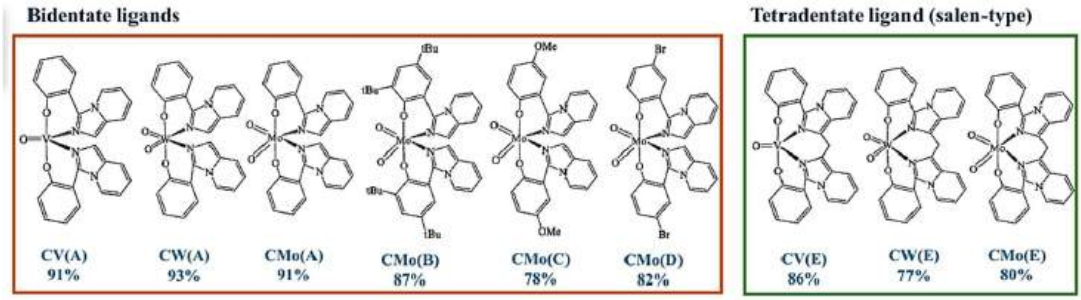

Fig. 1. Structures of bidentate and tetradentate imidazopyridine Mo(VI), W(VI), and V(IV) complexes.

All complexes displayed good catalytic performance in the epoxidation of cyclic olefins such as cis-cyclooctene, cyclohexene, S-limonene, and cyclooctadiene under mild reaction conditions, particularly in chlorinated solvents such as dichloromethane and chloroform. In contrast, lower conversions were observed for aliphatic olefins such as 1-hexene and for more sterically hindered substrates such as norbornene. These results highlight clear structure–reactivity relationships within this family of metal–imidazopyridine complexes and provide valuable insights for the rational design of efficient epoxidation catalysts.

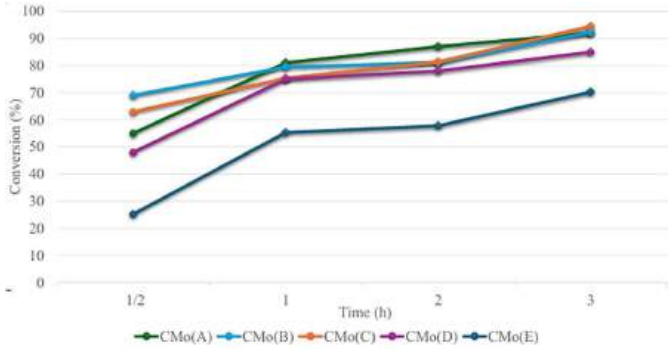

Fig. 2. Catalytic performance of imidazopyridine-based Mo(VI) complexes in olefin epoxidation under optimized conditions.

CCS - D3 - O10
Direct mechanocatalysis via catalytically coated milling tools

Maximilian Wohlgemuth[1], Lars Borchardt[1]
[1]*Ruhr-University Bochum, Germany*

Mechanochemistry uses mechanical force, such as grinding or milling, to drive chemical reactions, often without solvents. Direct mechanocatalysis builds on this by using milling components made of or coated with catalytic metals to perform reactions more sustainably. In this concept, the milling tools act as catalysts, combining energy input and catalytically active surfaces. Early approaches employed milling balls fully composed of catalytic metals. While effective, this method faced challenges due to the high cost of precious metals and the wear of milling balls. To address this, steel balls coated with thin layers (450 nm) of catalytic metals, like palladium, were developed.[1] This approach reduces the amount of precious metal required while maintaining catalytic activity and improving durability, allowing multiple uses with minimal catalyst loss (<1 ppm). Mechanistic studies confirmed that these reactions occur directly on the coated metal surfaces rather than via abraded catalyst species. The thin catalyst layer was sufficient to perform various cross-couplings, hydrogenation reactions, and oxidation reactions, in which metals such as palladium, gold, or rhodium were used cost-effectively. [2-4] Milling-medium-free approaches demonstrated that substrate–vessel contact alone can be sufficient for catalytic reactions in resonant acoustic mixers, which allowed the same catalyst layer to be used for over twenty reactions.[5] Most notably, palladium-coated screws and barrels enabled the first continuous direct mechanocatalysis in a twin-screw extruder, representing an important step toward scalable and continuous mechanochemical catalysis.[6]

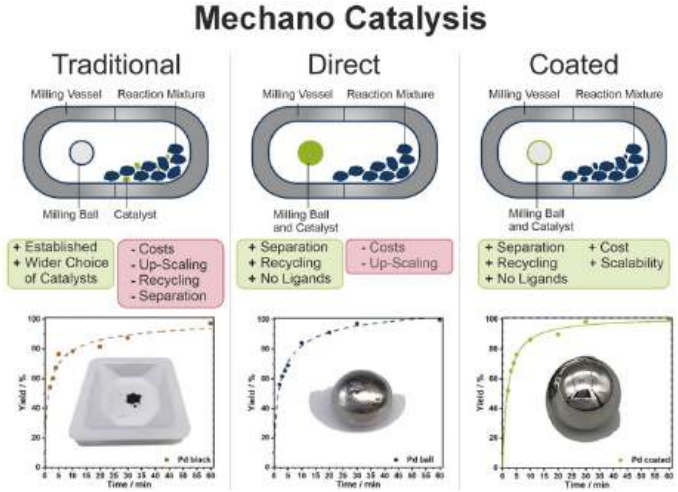

Fig. 1. Evolution of direct mechanocatalysis.[1]

[1]Wohlgemuth M.; Mayer, M.; Rappen M.; Schmidt F.; Saure R.;Grätz, S.;Borchardt, L. *Angew. Chem. Int. Ed*. **2022**, 61, e202212694.
[2]Wohlgemuth, M.; Schmidt, S; Mayer, M.; Pickhardt, W.; Graetz, S.;Borchardt, L. *Angew. Chem. Int. Ed.* **2024**, 63, e202405342.
[3]Wohlgemuth, M.; Mayer, M.; Straub, A. S.; Grätz, S.;Borchardt, L. *Angew. Chem. Int. Ed*. **2025**, e202424139.
[4]Wohlgemuth, M.; Schmidt, S.; Beißel, L.; Borchardt, L. *Chem. Commun*. **2025**, 61, 18838–18841.
[5]Wohlgemuth, M; Schmidt, S.;Mayer, M.; Pickhardt, W.; Grätz, S.; Borchardt, L. *Chem. Eur. J.* **2023**, 29, e202301714-
[6]Chantrain, V.; Rensch, T.; Pickhardt, W.; Grätz, S.; Borchardt, L. *Chem. Eur. J.* **2024**, 30, e202304060.

CCS - D3 - O11

Bio-electrocatalytic cascade processes for efficient valorization of biomass and plastic waste feedstocks into olefins

Christian M. Pichler[1], Richard Buchinger[1], Yashraj Kumar Singh[1]
[1]TU Wien, Institute for Applied Physics, Vienna, Austria

Olefins are important feedstocks in the chemical industry that are currently exclusively produced from fossil resources. The electrochemical oxidative decarboxylation of carboxylic acids, such as succinic acid or propanoic acid, can offer an environmentally friendly route to generate olefins provided the electrolysis uses renewable electricity and the acids are obtained from waste streams. We have developed several different approaches for the sustainable production of olefins from waste substrates.

The processes combine biocatalytic pretreatments with an electrocatalytic conversion, that can convert biomass waste or polyester wastes into defined olefins (e.g. ethene) as main product. In the process, dicarboxylic acids are central intermediates that undergo electrochemical reactions forming ethene as value added final product. With spectroscopical and electroanalytical approaches as well as quantum mechanical calculations, insights into the reaction mechanism could be gained as well. In this context the structure and composition of the electrochemical double layer demonstrated to be of vital importance for controlling yield and selectivity towards the olefin products. By adapting electrolyte composition and pH values, and supported by molecular dynamic calculations, optimal interface structures were determined to maximize product yield. Furthermore, different electrocatalysts were tested and material characteristics, beneficial for the olefin formation could be determined. [1]

Our results show that different types of wastes can be efficiently converted in coupled bio-electrochemical processes into value added olefin products. This is of great significance as it enables chemical recycling prospects at low temperatures and mild conditions towards defined gaseous products. Furthermore, it opens the possibility to obtain olefins in a sustainable way, and therefore offering one of the few alternatives to the current fossil-based olefin production routes.

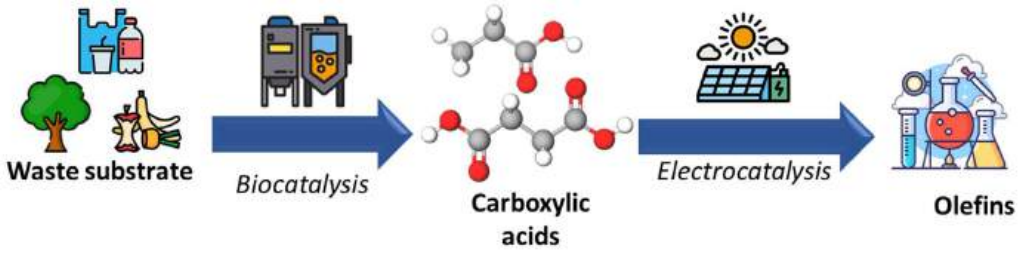

Fig.1. Schematic illustration of cascade process

[1]ChemSusChem, **2025**, 18, 10, e202402515

CCS - D3 - O12

Towards the direct reduction of atmospheric CO_2: Copper(I)-mediated hydrosilylation of highly diluted CO_2

Maël Bressoux, Thibault Cantat, Emmanuel Nicolas
Université Paris-Saclay, CEA, CNRS, NIMBE, France

Given our long-term dependence on carbon-based products, it will be crucial to capture carbon in the form of dilute CO_2 from the atmosphere and transform it into value-added products. However, in the current direct air capture (DAC) technologies, CO_2 at 400ppm must be concentrated using highly-energy intensive processes before its conversion.[1] Thereby, in order to create sustainable molecules with the highest frugality and to avoid this concentration energetic step, a promising solution is to develop robust catalytic system that can perform CO_2 reduction at very low partial pressure.

To date, CO_2 reductive reaction processes are using mostly H_2 as a reductant, resulting in high pressure conditions and additional energetic cost.[2] Therefore, we were interested in using hydrosilanes, as they are kinetically more active and are also stronger reducing agents than H_2. Additionally, their mild reduction potential is a significant advantage to achieve efficient reduction while minimizing energy losses.[3] A very efficient and active catalyst reported so far for the homogeneous hydrosilylation of CO_2 is the copper(I) hydride complex [(dppbz)CuH].[4]

In this communication, we present the catalyst optimization and its performance in the reduction of CO_2 at very low partial pressure (< 1% at 1 atm) using hydrosilanes. The [(dppbz)CuH]/$Me(OEt)_2SiH$ catalytic system, supported by preliminary mechanistic investigations, has been identified as a promising solution for the valorization of atmospheric CO_2 . Under ambient conditions, more than 80% conversion to silyl formate was achieved within 2 h. Additional results in the presence of oxygen revealed that the amount of hydrosilane will be a key factor for preserving reactivity under atmospheric conditions.

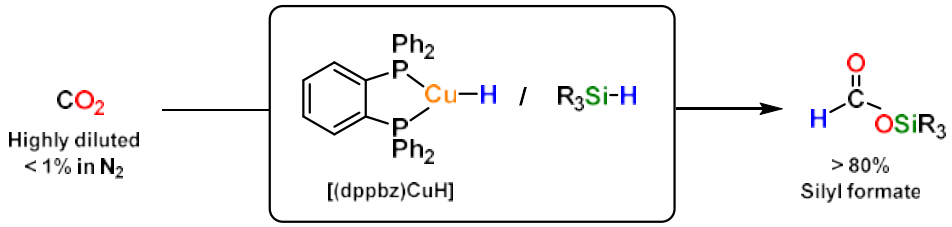

Fig. 1. Direct Reduction of Highly Diluted CO_2 with hydrosilane catalyzed by [(dppbz)CuH]

[1]Sanz-Pérez, E. S.; et al. *Chem. Rev.* **2016**, *116*, 11840–11876.
[2]Ye, J.; et al. *Science* **2025**, *387*, eadn9388.
[3]Chauvier, C.; Cantat, T. *ACS Catal*. **2017**, *7*, 2107–2115.
[4]Motokura, K.; et al. *Chem. Eur. J*. **2013**, *19*, 10030–10037.

CCS - D3 - O13
Operando Raman insights into TiO_2-supported metal catalysts for CO_2 hydrogenation

Guillaume Clet[1], Canio Scarfiello[2], Philippe Serp[2,3]
[1]Université Caen Normandie, ENSICAEN, CNRS, Laboratoire Catalyse et Spectrochimie, France; [2]Laboratoire de Chimie de Coordination, CNRS-UPR 8241, Université de Toulouse, France; [3]Institut Universitaire de France (IUF), Paris, France

Metals supported on various oxides are widely used as catalysts for CO_2 reduction. While *operando* IR studies have probed their role in reaction mechanisms, the dynamic evolution of the catalyst, particularly the support, remains underexplored. Nevertheless, the supported metals and the oxygen vacancies of the support which can be formed via H-spillover, can jointly induce phase transformations, participate in SMSI or contribute to the reaction. However, unlike ceria supported catalysts which are often characterized due to specific Raman bands, the study of oxygen vacancies on titania is less straightforward and only appears as a side effect on TiO_2 main vibrations.
Raman spectroscopy was therefore employed to characterize metals (Co [1] or Ru) supported on TiO_2 used as catalysts for CO_2 methanation. Their evolution was followed during reduction under H_2, under reaction conditions with H_2/CO_2 and also under pure CO_2. As expected, initial treatment in hydrogen alters the metal precursors, but interestingly, the impact on TiO_2 support and its evolution differ between Co and Ru catalysts. New oxygen vacancies were detected on the support by Raman in presence of cobalt, whereas reduction primarily affected Ru, which migrated toward the support when temperature was increased. Upon treatment under CO_2, cobalt particles were re-oxidized, which also affected the involvement of oxygen vacancies, and a new phase $CoTiO_3$ was observed. The *operando* characterization showed a limited impact of the H_2/CO_2 reaction mixture on Co/TiO_2 while in the case of Ru/TiO_2, the catalytic behavior and the catalyst were modified depending on the pre-reduction treatment.
The evolution of both Co and Ru metals supported on titania can thus be discriminated by *operando* Raman. The evolution of the support and its oxygen vacancies evolved distinctly on these catalysts either during the initial reduction, during CO_2 hydrogenation reaction or also under pure CO_2.

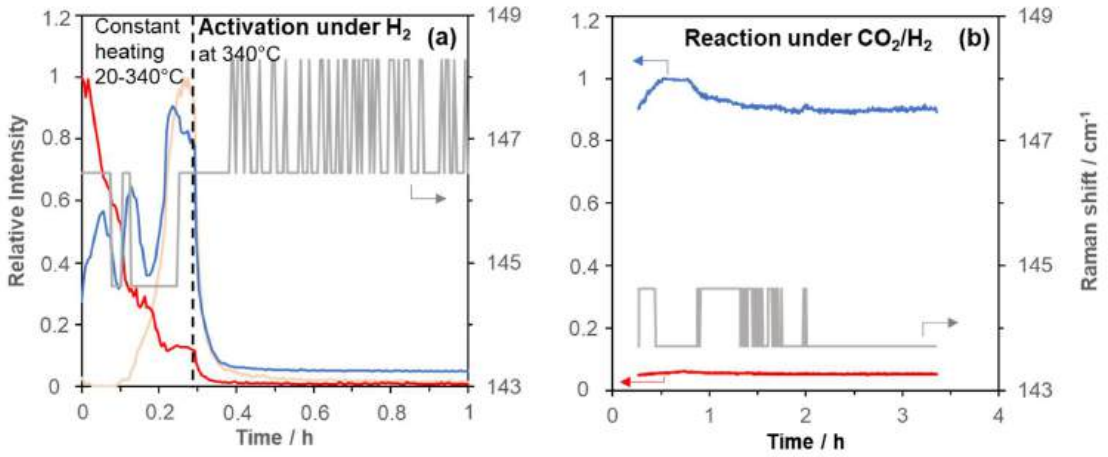

Fig. 1. Raman characterization of Co/TiO_2 under (a) Activation under H_2 ; (b) Reaction under CO_2/H_2.
Grey curve (right scale) reports the Raman shift of the Eg band of TiO_2 at 145 cm^{-1} while the other curves (left scale) report the relative intensities referred to the corresponding maximum intensity at each step: Blue curve: TiO_2 band at ca. 145 cm^{-1}; Red curve: band at ca. 680 cm^{-1} characteristic of CoO_X species; Orange curve (in (a)): band at 1000-1600 cm^{-1} characteristic of carbonaceous species

[1]Durupt, A.; Scarfiello, C.; Schmidt, L.; Minh, D. P.; Soulantica, K.; Meunier, F.; Ersen, O.; Zafeiratos, S.; Clet, G.; Serp, P. *ChemCatChem* **2026**, *18* (1), e01392

CCS - D3 - O14
Bimetallic Ni-Cu and Cu-Pd (de)hydrogenation catalysts – Composition and particle size effects

Petra de Jongh
Deby Institute for Nanomaterials Science & Institute for Sustainable and Circular Chemistry, Utrecht University, The Netherlands

Supported metal nanoparticles of Pd and Ni are active (de)hydrogenation catalysts, but often do not present a combination of all desired catalytic properties, which comprise not only catalytic activity, but also catalyst selectivity and stability. Strategies to tune catalyst properties are to play with the particle size, use support effects and to alloy with a second metal which often leads to synergetic properties. It is specifically interesting to combine these very active hydrogenation catalyst metals with one of the coinage metals, Cu, Ag or Au, which are not the most active elements, but can steer the selectivity towards desired products.
In this presentation I will in detail discuss two examples from recent work in our own group.[1-2] A first example concerns Pd-based catalysts for the selective hydrogenation for the removal of polyunsaturated hydrocarbon traces from alkene feedstocks. The second example deals with Ni-based catalysts for the decomposition of methane into H_2 (a fuel that does not emit CO_2 upon combustion) and valuable carbon nanostructured materials. Our results highlight the importance of combining statistically relevant (operando) characterization and catalytic tests with microscopic information on individual nanoparticles to understand catalytic trends.

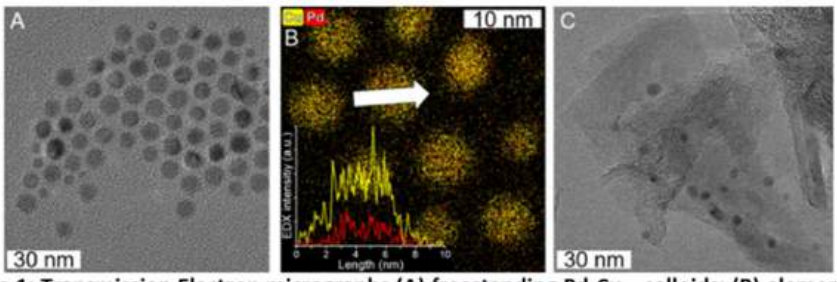

Figure 1: Transmission Electron micrographs (A) freestanding Pd_3Cu_{97} colloids; (B) elemental mapping showing coexistence of Pd and Cu in individual nanoparticles and (C) After deposition onto a graphite nanoplatelets support

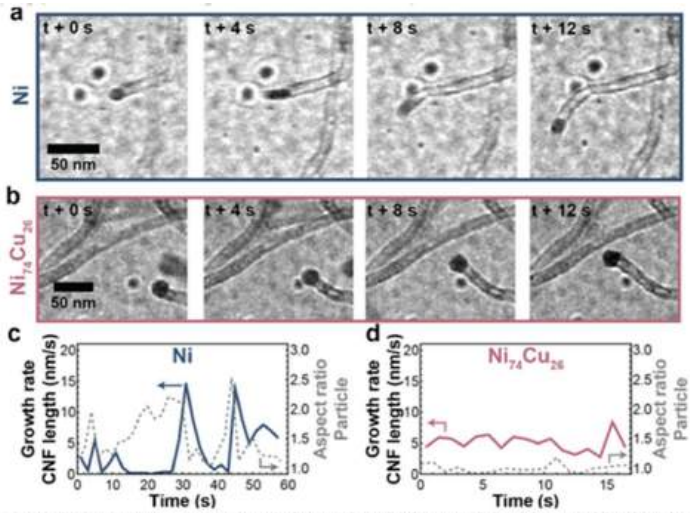

Figure 2: Carbon nanostructure growth from Ni and NiCu particles observed in the electron microscope; snapshots of structures grown by a (a) Ni and (b) NiCu (26 wt% Cu) nanoparticle.

[1]O. E. Brandt Corstius et al., J. Catal. **2023**, 427, 115103; *React. Chem. Eng*. **2024**, DOI:/10.1039/D4RE000
[2]S.E. Schoemaker, T.A.J. Welling et al. Catal. Today **2023**, 418, 114110; J. Phys. Chem. C. **2023**, 127, 15766-15774.; *Mater. Adv.* **2024** DOI: 10.1039/D4MA00138A

CCS - D3 - O15

Robust ink-formulated single-atom catalyst electrodes for anodic and cathodic organic electrosynthesis

Milla Viglienco[1], Jai White[2], Helena Lundberg[2], Gianvito Vilé[1]*
[1]Politecnico di Milano, Italy; [2]KTH Royal Institute of Technology, Sweden

The growing interest in organic electrosynthesis calls for electrode materials that can withstand the harsh conditions imposed by organic reaction media. Despite significant progress in catalyst development, the limited robustness of electrode materials continues to hinder efficiency and reproducibility.[1] Here, we have investigated metal single-atom catalysts ($M_1@CN_x$, where M = Ag, Ni) formulated as inks and deposited on diverse electrode supports, evaluating their robustness under both anodic and cathodic organic electrosynthetic conditions (Figure 1a).

Following optimization of the catalyst inks, including assessment of polymeric binder stability in organic solvents and standardization of deposition reproducibility by drop casting, we conducted cyclic voltammetry on multiple ink formulations. These measurements allowed us to select transformations that exhibited characteristics inner-sphere mechanisms. We selected the reduction of benzyl bromide and the oxidation of benzyl alcohol as representative cathodic and anodic reactions, respectively. For both reactions, $M_1@CN_x$-modified electrodes outperformed conventional graphite electrodes while maintaining excellent integrity of the deposited catalyst layer. Specifically, $Ag_1@nCN_x$-based electrodes increased the mass balance of benzyl bromide reduction products by *ca.* 20% compared to bare graphite. In the oxidation of benzyl alcohol, the presence of metal active sites doubled the yield of the oxidative products. Notably, we observed that the polymeric binder played a decisive role on the catalyst performance: NAFION enhanced the activity of $Ni_1@mpgCN_x$, whereas PEDOT:PSS improved the activity of $Ag_1@mpgCN_x$. These results highlight the potential of tunable electrode/catalyst/binder combinations as alternatives to conventional electrodes, contributing to more versatile electrosynthetic setups. Moreover, the low-cost and simple deposition methods used here can be readily translated to the preparation of electrodes for flow electrochemical system.[2]

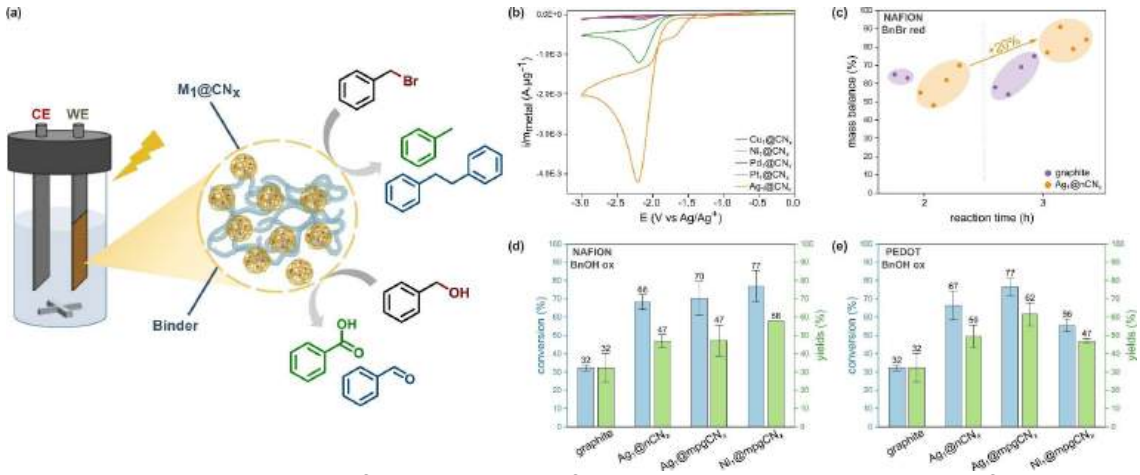

Fig. 1. (a) Reactions schemes for the reduction of benzyl bromide and the oxidation of benzyl alcohol, **(b)** cyclic voltammogram for the reduction of benzyl bromide on different catalyst inks, **(c)** mass balance of benzyl bromide reduction products overtime for bare graphite and $Ag_1@nCN_x$ on graphite cathodes, **(d)** comparison of catalytic activities of various NAFION-based inks and **(e)** various PEDOT-based inks on the benzyl alcohol oxidation.

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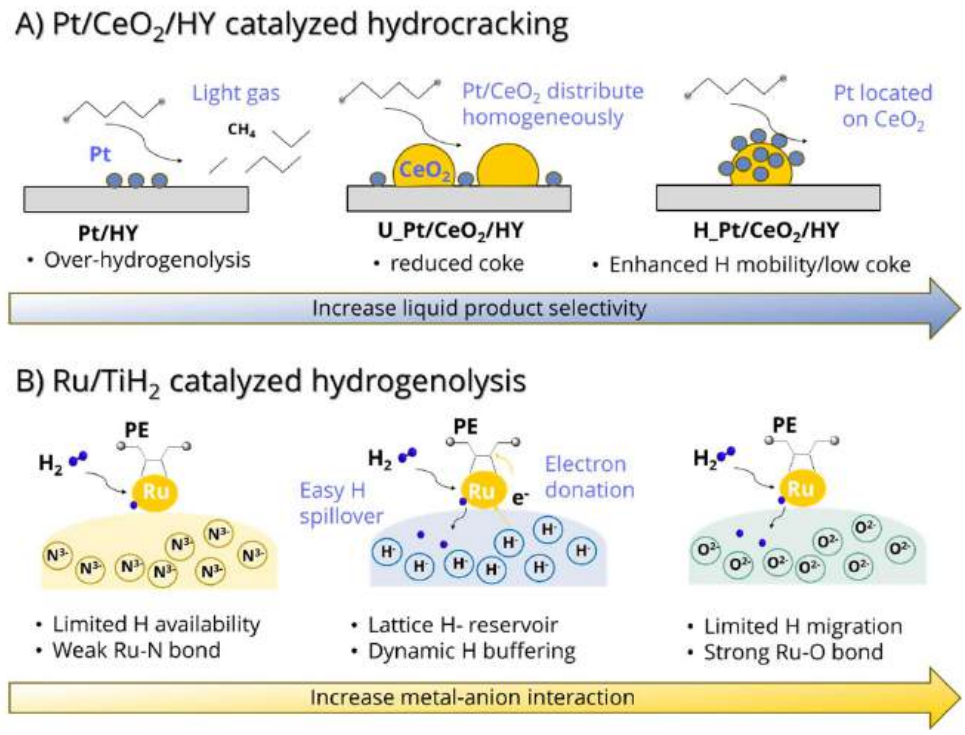
CCS - D3 - O16
Hydrogen regulation at metal–support interfaces for selective plastic hydrogenolysis

Yu Cao, Bert Weckhuysen*
Institute for Sustainable and Circular Chemistry, Utrecht University, The Netherlands

Catalytic hydrogenolysis has emerged as a powerful strategy for the upcycling of polyolefin plastics, enabling the decomposition of inert C–C backbones into value-added liquid hydrocarbons under milder conditions than conventional pyrolysis.[1] A central challenge lies in controlling product selectivity, i.e., suppressing over-hydrogenolysis and low-value light gas formation while maximizing liquid-range products.[2] Hydrogenolysis selectivity has been reported to be governed by metal–hydrogen dynamics at the metal–support interface, where efficient internal C–C scission requires sufficiently high surface hydrogen coverage and rapid hydrogenation–desorption of alkyl intermediates.[3] Here, we address this challenge by manipulating hydrogen availability at the metal–support interface through two complementary catalyst design strategies. In the $Pt/CeO_2/HY$ system, spatially confined CeO_2 nano-islands electronically modulate Pt and influence hydrogen mobility across the metal–oxide–zeolite interface, enabling controlled hydrocracking while effectively suppressing coke formation and enhancing catalyst stability. In contrast, the Ru/TiH_2 system exploits lattice hydride species as intrinsic hydrogen reservoir. Reversible hydride-to-metal charge transfer stabilizes electron-rich $Ru^{\delta-}$ centers, dynamically buffering surface hydrogen availability and promoting efficient internal C–C bond cleavage while minimizing over-hydrogenolysis and methane formation. Together, these results establish framework for hydrogen regulation at metal–support interfaces, offering new insights into dynamic metal-support interaction for next-generation catalysts in sustainable plastic hydrogenolysis.



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CCS - D3 - O17

Magnetically induced iron-catalyzed hydrodeoxygenation of benzylic esters and polyesters

Sihana Ahmedi,[1,2] Lise-Marie Lacroix,[3,4] Derya Demirbas,[1] Daniel J. SantaLucia,[1] Claudia Weidenthaler,[5] Walid Hetaba,[1] Walter Leitner,[1,2] Alexis Bordet[1*]

[1]Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany; *[2]Institute of Technical and Macromolecular Chemistry RWTH Aachen University, Aachen, Germany*; *[3]Université de Toulouse, Laboratoire de Physique et Chimie des Nano-Objets, Toulouse, France*; *[4]Institut Universitaire de France (IUF), Paris, France*; *[5]Max-Planck für Kohlenforschung, Mülheim an der Ruhr, Germany*

Exhaustive reduction of esters to methyl-containing compounds is challenging but of fundamental importance for enabling degradation and recycling of polyesters and the synthesis of methyl and tolyl derivatives in synthetic chemistry.[1-2] Conventionally, this transformation relies on non-sustainable pathways, employing excess of strong and often hazardous reducing agents (e.g. metal hydrides, hydrosilanes, ammonia borane) under harsh conditions.[2-3] As a result, the development of catalytic and atom-economical ester reduction pathways using H_2 as a reducing agent under mild conditions is highly desired, but remains a challenge.

Herein, we explore the selective ester reduction with H_2 using iron-based nanoparticles (NPs) with magnetic heating capabilities.[4] Magnetic induction heating has been demonstrated by our group and others to heat suitable catalyst materials in a very rapid, localized, and energy efficient manner.[5-9] This technology obviates the necessity of heating the entire reactor environment, potentially leading to lower overall process temperatures and reduced energy consumption. In the present work, we prepare and characterize iron carbide nanoparticles (ICNPs) with exceptional induction heating capabilities, and apply them to the magnetically induced hydrodeoxygenation of benzylic esters using H_2.

ICNPs were prepared following an organometallic approach[6] and fully characterized. ICNPs were activated by magnetic induction heating and exhibited high activity, selectivity, and stability for the hydrodeoxygenation of a large scope of esters and polyesters (including real-life PET) into tolyl derivatives under mild conditions (3 bar H_2, 200 °C).[4] The catalyst's adaptivity to intermittent power supply was demonstrated by regularly stopping and re-starting the AC magnetic field. Strikingly, ICNPs heated conventionally (200 and 350 °C) showed poor activity and stability. This work may pave the way toward practical implementation of ester hydrodeoxygenation in research and industry, and demonstrates the broad potential of the emerging field of magnetically induced catalysis for synthetic transformations typically requiring demanding operating conditions.

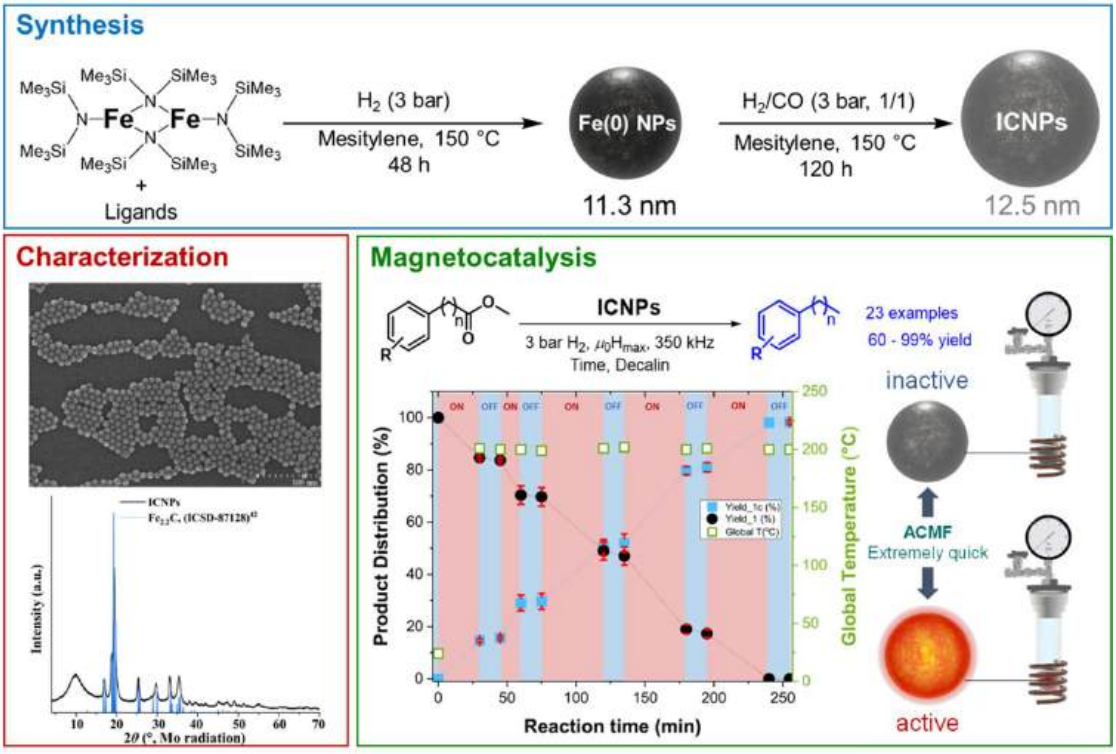

Fig. 1. Illustration of the approach, with the synthesis of ICNPs, their characterization, and their application to the magnetocatalytic reduction of benzylic esters.

The authors thank Jan Ternieden (Max-Planck-Institut für Kohlenforschung) for PXRD measurements, John-Tommes Krzeslack (MPI-CEC) for XPS measurements, Norbert Pfaender (MPI-CEC) for TEM and SEM-EDX measurements, and Annika Gurowski, Alina Jakubowski, and Justus Werkmeister (MPI-CEC) for GC and GC-MS measurement support. We thank the Max Planck Society and the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – Exzellenzcluster 2186 “The Fuel Science Center” ID: 390919832 for financial support.

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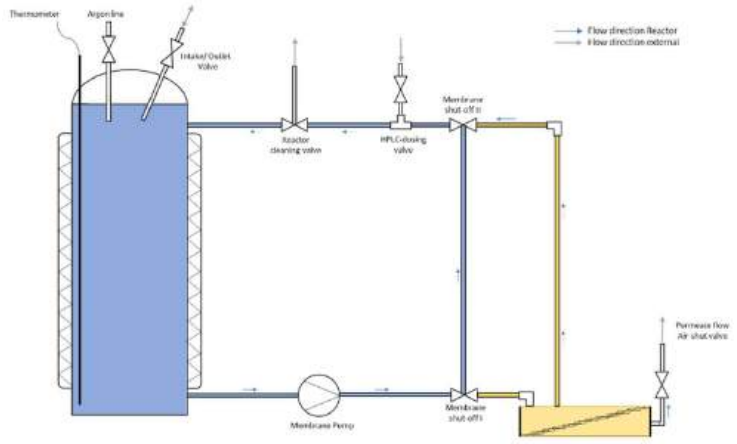
CCS - D3 - O18
Reduction of levulinic acid to GVL – Catalyst recycling through membrane nanofiltration

Lars Faber, Lan Le Hoang, Murielle Rabiller-Baudry, Cédric Fischmeister
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes), France

With the arising interest in transitioning from fossil fuels to more renewable resources, new strategies have to be investigated and developed. In that context catalysis and catalyst design marks one of the major challenges to overcome for aforementioned transition.[1,2] However, as of now, the re-usability of homogeneous catalysts marks one of the major disadvantages for the use of homogeneous catalysts in industry,[3,4] where catalysts are either single use, or their structural integrity is purposely destroyed to recover the metal only. In either case, purification of the product or recycling of the catalyst requires immense amounts of energy and resources. Hence, industry tends to prefer heterogenous systems, despite their oftentimes lower efficiency and selectivity.[5]
Circumventing those disadvantages,membrane nanofiltration presents a novel alternative to enable catalyst separation from the reaction media.[6] Additionally, membrane nanofiltration holds immense potential in lowering the carbon footprint of reactions, due to much lower energy requirements compared to traditional techniques, such as distillation.[7]
This project aims to implement nanofiltration as efficient alternative to implement catalyst re-use in homogeneous catalysis, combining the re-usability of the catalyst with the increased selectivity provided by homogeneous systems. For this purpose, a lab-scale membrane nanofiltration system was planned (Scheme 1), built, and applied for the base-free iridium-catalyzed transfer hydrogenation of levulinic acid towards γ-valerolactone in a batchwise reactor under mild conditions.[8,9]



Scheme 1: Schematic depiction of the planned reactor setup for the iridium-catalyzed, base-free transfer hydrogenation of levulinic acid from biomass to γ-valerolactone.

Followed by the planning of the setup, extensive membrane testing and parameter optimization allow the efficient separation of the reaction product from the catalyst, retaining its activity over several cycles. Extensive analytical monitoring of the reactor and its feeds and products revealed catalyst leaching in the low ppm-region.

We are grateful for the funding through the PEPR-SPLEEN ECOCHEM project within the France2030 plan.

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CCS - D3 - O19

Steric hindrance of proton donor modulates heterogeneous electrochemical nitrogen reduction reaction selectivity in non-aqueous electrolyte

Dongmin Park[1], Changhyeok Choi[2], Jinyoung Ko[1], Yousung Jung[1]
[1]Seoul National University, South Korea; [2]University of Toronto, Canada

Ammonia is a very important chemical used across various industries. The conventional Haber-Bosch (HB) process to produce ammonia has a large carbon footprint, let alone the harsh operating conditions being responsible for huge energy consumption.[1] Another problem lies in grey hydrogen being the main source of H_2 for the HB process, where steam reforming of fossil fuels is utilized. Considering these concerns regarding ammonia production, there is urgent need for alternative production methods.
The electrochemical nitrogen reduction reaction (NRR) offers a sustainable alternative to conventional methods of ammonia production.[2] Electrochemical nitrogen reduction reaction (NRR) in aqueous electrolytes suffers from a premature decline in activity due to dominant hydrogen coverage at cathodic potentials, inhibiting nitrogen adsorption and facilitating the hydrogen evolution reaction (HER).[3] Leveraging the steric hindrance of proton donors in aprotic solvents could selectively suppress the HER while maintaining NRR activity. Using computational methods, we show that increasing proton donor steric hindrance limits the kinetics towards the HER while it insignificantly affects the NRR. This originates from the steric-dependent accessibility of the proton to the acceptor site where metal surface sites have inhibited access in the existence of bulky alkyl groups. This understanding between PCET kinetics and steric-dependent mechanisms will provide a guide to facilitate new electrolyte designs for electrochemical reactions.

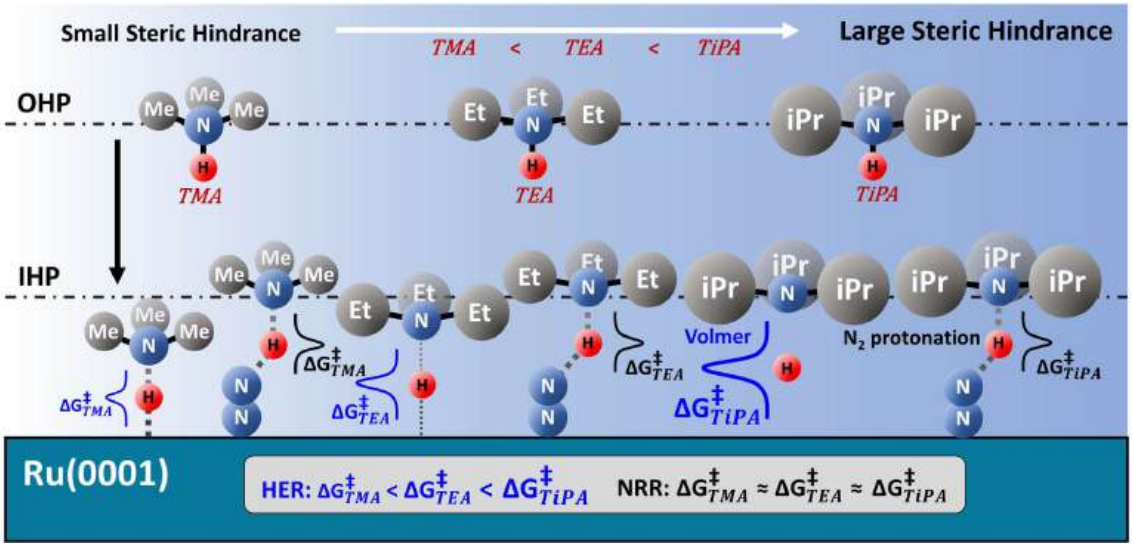

Fig. 1. Schematic overview of this work.

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CCS - D3 - O20

Atomically dispersed Ru on zeolite catalysts for unlocking the potential of the biobased *cis,trans*-muconic acid

Ibrahim Khalil[1,2], Marco Giulio Rigamonti[1], Lisa De Vriendt[1], Michiel Dusselier[1]
[1]Center for sustainable Catalysis and Engineering, KU Leuven, Belgium; [2]IRCELYON, CNRS, France

Muconic acid (MA) presents 3 isomeric forms: *cis,cis*- and *cis,trans*- (*ct*) that can be obtained from biobased sources, and the value-added *trans,trans*-isomer (*tt*). This latter consists a platform molecule for synthesizing several derivatives such as **(1)** adipic acid via hydrogenation reaction, **(2)** hexenedioic acid via mono-hydrogenation, and **(3)** terephthalic intermediate via the Diels-Alder cyclo-addition (**Figure 1**).[1] The biotechnological synthesis of MA from glucose produces often the *ct*MA, making the development of an isomerization step towards the *tt*-isomer very essential. In this work, we present the several explored routes that we investigated for the isomerization of *ct*-muconates (e.g., solvent driven and Ru-based isomerization), with a highlight on their strength and weaknesses.[2,3] In addition, we also present our first findings on the Ru-based selective mono-hydrogenation of muconic esters to produce **(2)**.

Isomerization: a 95% selectivity towards the *tt*-isomers could be achieved together with high productivity values for the different explore isomerization methods. In the Ru-based catalysts, a TON exceeding 2500 mol_{MA}/mol_{Ru} could be achieved. Moreover, the in-depth characterization of the catalyst was conducted (EXAFS, ICP, H_2-TPR, FT-IR, BET) to confirm the atomic distribution of Ru atoms and elucidate the reaction mechanism. Finally, a *one-pot* isomerization/Diels-Alder reaction was conducted to produce **(3)** and was successful with different ester forms.

Mono-hydrogenation: To date, the synthesis of **(2)** was only reported using electrochemical methods.[4] **(2)** can serve as a co-monomer in the synthesis of unsaturated polyamides, opening routes for the functionalization of these latter. The difficulty in making **(2)** remains in the control of the hydrogenation step which usually end up with the formation of adipic acid **(1)**. Here, we report the tuned Ru on zeolites as efficient and selective hydrogenation catalysts, in an H_2-free system, to obtain the desired product **(2)** in yields surpassing the 50% and selectivity around 70%.

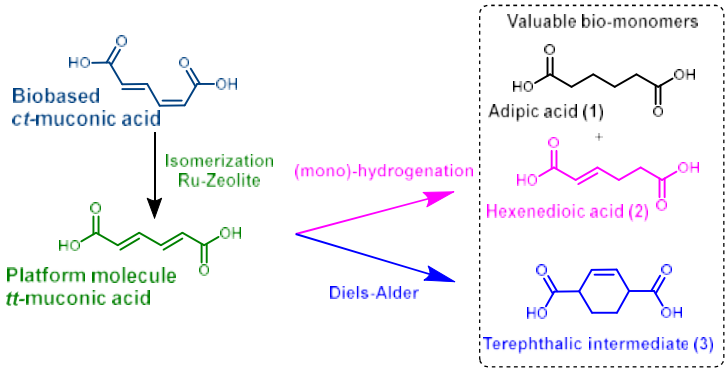

Fig. 1. Reactions scheme for the isomerization of *ct*-muconic acid using Ru-zeolite catalyst followed by the different valorization routes of the *tt*-isomer (hydrogenation and Diels-Alder reactions).

Acknowledgements: This work was funded by FWO foundation for postdoctoral research (grant number 1260321N for I.K.) and the Catalisti cSBO project C2O with support of VLAIO (HBC.2020.2611).

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CCS - D3 - F01

Multi-faceted insight into the thermochemical redox behaviour of manganese-oxide-based model catalyst, $Na_2Mn_3O_7$ – Comparative analysis through DFT, operando TEM and XAS

Karol Górecki[1,2], Monika Fedyna[2], Anna Wach[3], Michał Śliwa[3], Zbigniew Sojka[2], Joanna Gryboś[2]
[1]Doctoral School of Exact and Natural Sciences, Jagiellonian University in Kraków, Poland; [2]Faculty of Chemistry, Jagiellonian University in Kraków, Poland; [3]National Synchrotron Radiation Centre SOLARIS, Jagiellonian University in Kraków, Poland

Catalysts are essential for our ever-developing society, as they enable crucial reactions at attainable conditions. Among them, transition metal oxides play a central role in technologies relying on reversible redox processes, including energy storage, fuel production, and environmental remediation. An example of environmentally benign and effective catalysts are manganese oxides, especially modified structures containing aliovalent manganese atoms which can easily be oxidised or reduced. Recently, a lot of research has been put into catalysts with alkali atoms[1], which stabilise and promote mixed valence of manganese, including $Na_2Mn_3O_7$, characterised by a layered morphology[2]. However, this same chemical flexibility also leads to complex structural and electronic changes during redox cycling, making it challenging to establish clear relationships between atomic-scale structure and macroscopic performance.
In this contribution, we present a comprehensive, multi-technique investigation of the layered manganese oxide $Na_2Mn_3O_7$ as a model catalyst system, combining state-of-the-art operando S/TEM-EELS, O-XAS, and DFT calculations, aimed at elucidating the mechanism of reversible redox reactions. Ex-situ electron microscopic analysis on an euhedral sample (**Fig. 1a-b**) allowed for determination of morphology and exposed facets, which were then used for analysis of oxygen vacancy formation through DFT (**Fig. 1c**). Operando measurements facilitated monitoring of structural evolution upon reduction and reoxidation, expressed predominantly through changes in oxidation states (shifting of Mn-$L_{2,3}$ lines in EELS and shape changes of the XAS spectrum – **Fig. 1d**). Through a combination of ex-situ and operando experiments with the DFT results, it was possible to identify a temperature window where the catalyst exhibited reversible redox behaviour, concurrently with stable structure and morphology. This comprehensive approach contributes to a deeper understanding of redox processes occurring in the Mn-based catalysts and their potential applications in thermochemical cycles.

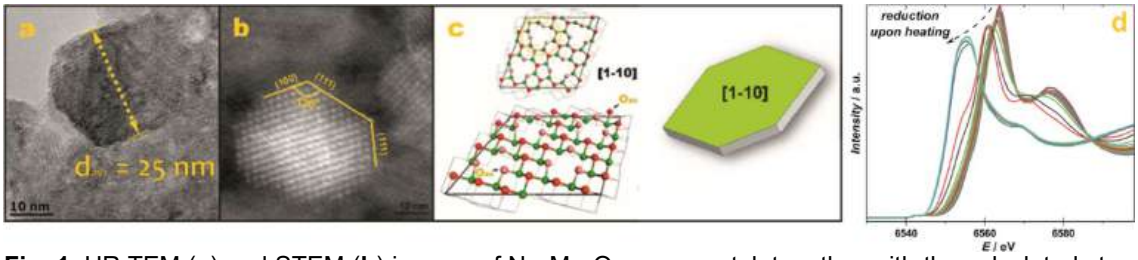

Fig. 1. HR TEM (**a**) and STEM (**b**) images of $Na_2Mn_3O_7$ nanocrystal, together with the calculated structure of the most abundant (1-10) surface and retrieved morphology (**c**). Operando XAS spectra of the Mn K-edge for $Na_2Mn_3O_7$ catalyst in an inert atmosphere upon heating from RT to 700 °C (**d**).

The research is carried out within the OPUS 25 (grant number 2023/49/B/ST4/00740, PI: Dr Joanna Gryboś) project, funded by NCN, the Polish National Science Centre. This research received support and funding from the program "Excellence Initiative – Research University" at the Jagiellonian University. Research at the National Synchrotron Radiation Centre SOLARIS was supported by the Ministry of Science and Higher Education, Poland, under contract no. 1/SOL/2021/2.

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CCS - D3 - F02

Tailoring Al-differentiated HZSM-5 Catalysts: A solution for controlled ethylene oligomerization and resistance to deactivation

Agata Olszewska[1], Julia Sobalska[1,2], Karolina Tarach[1], Oliwia Rogala[1,2], Kinga Góra-Marek[1]
[1]Faculty of Chemistry, Jagiellonian University in Kraków, Poland; [2]Doctoral School of Exact and Natural Sciences, Jagiellonian University in Kraków, Poland

Ethylene oligomerization produces key intermediates for fuel and petrochemical applications. HZSM-5 zeolites are attractive solid acid catalysts which performance strongly depends on the balance between acid site density and accessibility influencing activity, selectivity, and coke formation.

This study examines the effect of aluminum content in ZSM-5 (Si/Al = 15-140) on ethylene oligomerization. Catalyst performance was evaluated in two states: the initial reaction of the fresh catalyst (R) and after regeneration (R&Ox). All catalysts maintained high and stable ethylene conversion (>92%, Fig. 1A). Quantitative Py-FTIR revealed that reaction-induced coking reduces the number of both Brønsted (BAS) and Lewis (LAS) acid sites by approximately half. While oxidative regeneration fully restores BAS, the persistent deficit in LAS indicates irreversible transformation or incomplete recovery during TPO.

The C_3/C_4 ratio describes catalyst selectivity (Fig. 1B). While it is independent of the Si/Al ratio in fresh catalysts (R), regeneration induces a strong dependence. In R&Ox samples, increasing Si/Al leads to higher C_3/C_4, indicating a shift toward secondary reactions, i.e. cracking, isomerization, and hydrogen transfer. This is supported by increased fractions of $C_{4=}/C_4$ and *iso*-$C_{4=}/C_4$ products. Concurrently, lower aluminum content significantly enhances propene formation ($C_{3=}/C_3$), which more than doubles after regeneration. This performance is attributed an increase in BAS strength coupled with a diminished contribution from Lewis acid sites. GC–MS analysis showed that coke evolves from heavy polyaromatics in R to an intermediate C_7-C_{10} fraction in R&Ox at all Si/Al ratios.

Mechanistic insights were further enriched by MCR-ALS analysis. By resolving concentration profiles and pure spectra of spectroscopically active components, we demonstrated that the density and strength of acid sites rule both selectivity and catalyst lifetime. These findings underscore the importance of optimizing ZSM-5 architecture for enhanced olefin production.

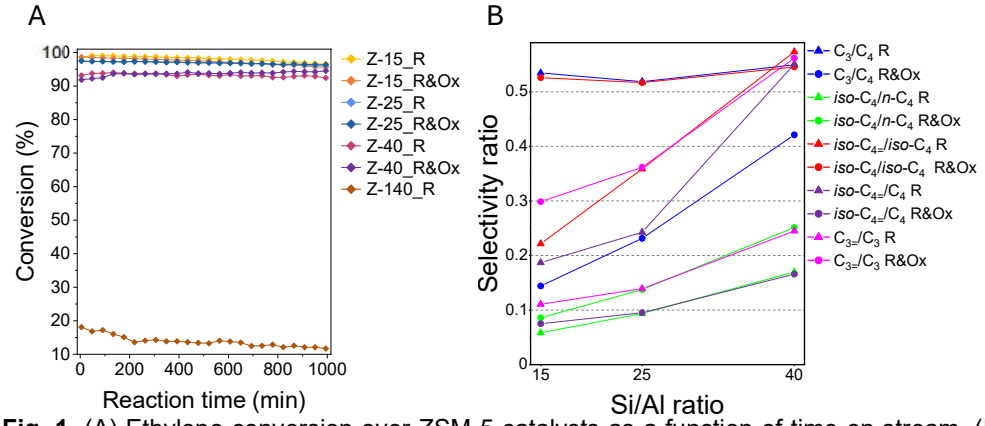


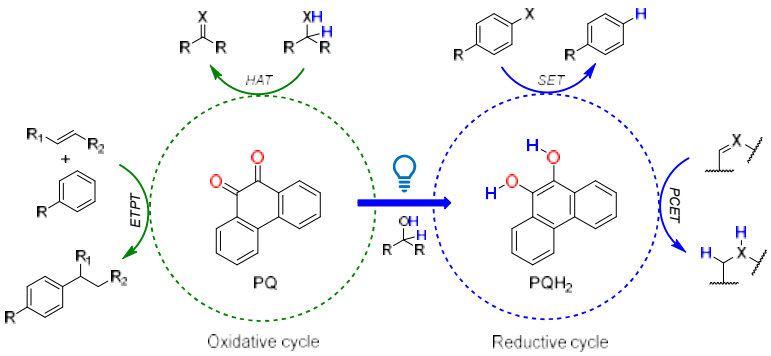
Fig. 1. (A) Ethylene conversion over ZSM-5 catalysts as a function of time on stream, (B) effect of the Si/Al ratio on product selectivity under R and R&Ox conditions.

The work was financed by Grant No. 2023/49/B/ST4/02340 from the National Science Centre, Poland.

CCS - D3 - F03
Phenanthrenequinones (PQs): Swiss army knife in photocatalysis

Andrés Mollar-Cuni[1,2] and Juho Helaja[1]
[1]University of Helsinki, Finland; [2]Universitat Jaume I (UJI), España

During the last decades, the development of photoredox catalysis has revolutionized the means of performing organic transformations. The use of organic dyes as photocatalyst, instead of classical metal-based photosensitizers, has increased interest in this methodology due to its availability and lower cost.[1] However, one well known weakness of the method is the requirement for (over)stoichiometric amounts of sacrificial oxidants/reductants, co-catalysts or additives, such as HAT agents, which produce both economic burden and chemical waste. In recent years, phenanthrenequinones (PQs) have emerged as promising catalysts due to its versatility, as it can act as direct HAT photocatalyst, as well as reacts through SET or ETPT mechanisms.[2] Additionally, phenanthrenehydroquinones (PQsH2), the reduced form of PQs which can be obtained in situ using secondary alcohols as hydrogen source, are good reductant photocatalyst proceeding via SET or PCET mechanism. In view of this versatility, PQs could be considered as Swiss army knife in photocatalysis.



PQs show incredible tuneability as their photochemical and photophysical properties are directly related with their structure. Tailoring of PQ with EWG-substituents (-CF_3) increases its excited state reduction potential and makes it a better photooxidant and, correspondingly, the tailoring of PQ with EDG-substituents (-OMe) makes its hydroquinone a superior photoreductant. In recent years, our group has developed a simple and efficient methodology to access PQ derivatives with different functionalities, such as EWG and EDG groups as well as π-extended framework or cationic functionalities. It allows the design of specific catalysts for each transformation obtaining more efficient and active photocatalytic systems.

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CCS - D3 - F04
Hydrogen bond donating large pore MOFs as catalysts

Christophe M.L. Vande Velde[1], Leili Esrafili-Dizaji[1]
[1]University of Antwerp, Faculty of Applied Engineering, Dept. of Biochemical and Chemical Technology, iPRACS, Belgium

In the quest for reusable active heterogeneous hydrogen-bond donating organocatalysts that are well-characterizable [1-3], we have prepared a multitude of large pore MOFs based on ditopic, tritopic and tetratopic urea and squaramide linkers (Fig. 1). We are presenting here the structures of some of the more interesting examples, as well as catalytic test data from a Friedel Crafts alkylation of (functionalized) indole with (functionalized) beta-nitrostyrene (Fig.2).

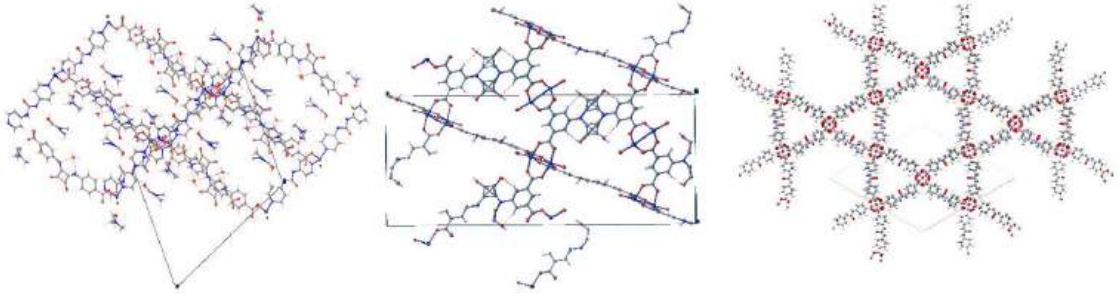

Fig. 1. Mixed urea-squaramide UA-157 and UA-143, and hexagonal channel-type urea-based UA-3

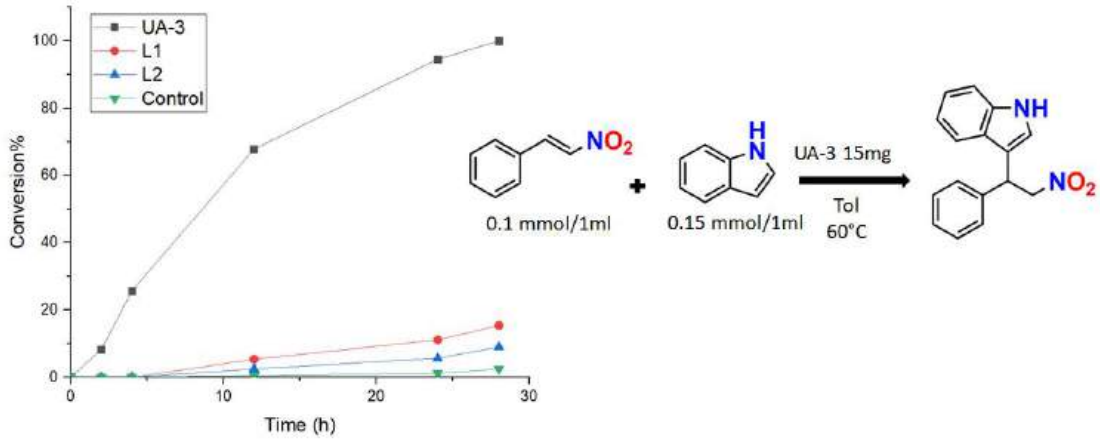

Fig. 2. Catalytic data on Friedel-Crafts test reaction with UA-3 as a catalyst

The authors thank the FWO Vlaanderen for the postdoctoral mandate of LE and the funding for the diffractometer via project I012324N.

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CCS - D3 - F06
Enabling technologies in flow chemistry for data-rich reaction optimisation

Diarmuid O'Hanlon[1,2], Brian Glennon[1], Marcus Baumann[2]
[1]APC Ltd, Dublin, Ireland, [2]UCD School of Chemistry, Dublin, Ireland

Over the past few decades, flow chemistry has emerged as a powerful tool for enhancing synthetic methodologies, drug discovery, and reaction development, owing to its advantages over traditional batch processes.[1] While standard flow setups consist of a pump, reactor tubing, and a collection vessel, the integration of additional technologies such as in-line PAT, in-line workup devices, and high-throughput tools offer significant further potential for optimisation, yet these still remain underutilised (Figure 1).

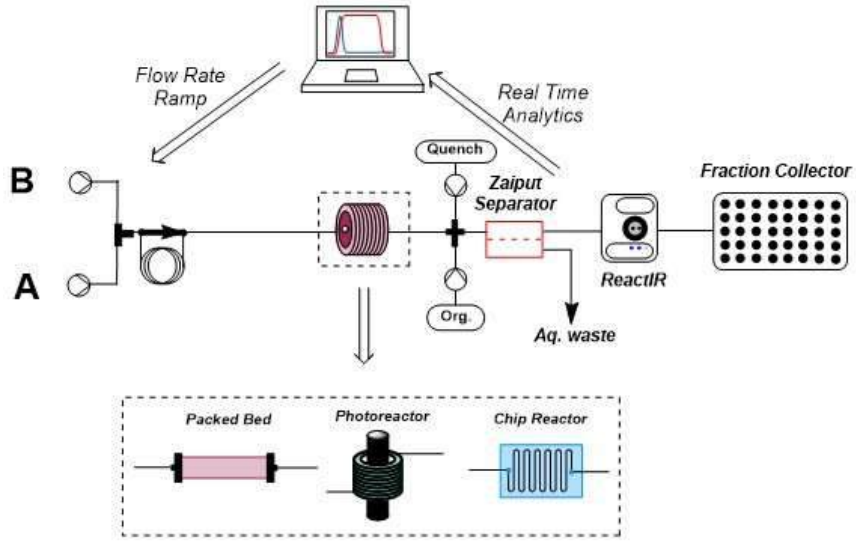

Fig. 1. Flow chemistry setup utilising advantages gained from inline analytical and workup tools.

This research demonstrates how the established advantages of flow chemistry can be exploited both to improve known batch reactions and to enable smart, efficient process optimisation, through carefully designed experimental strategies. By combining photoflow chemistry with in-line workup technologies, the aqueous Kochi–Salomon reaction developed by the Burns group[2] has been adapted to demonstrate that the [2+2] cycloaddition of unactivated olefins can be achieved in the absence of any Cu(I) catalyst.[3]
Further advantages of flow chemistry are realised through its inherent continuous processing-logic, which enables the use of in-line analytical techniques (e.g. IR), for data-rich optimisation. This approach facilitates intelligent experimental design, including optimisation strategies not possible in batch, such as Dynamic Flow Experimentation or "Close-The-Loop" optimisation via OPC communication between flow hardware and IR analytics. Collectively, these methods highlight the potential flow chemistry supplies towards reaction discovery and/or the rapid development of interesting drug-like scaffolds.

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CCS - D3 - F08

Getting all ducks in one row, unravelling the complexity of chemical recycling of hard-to-recycle plastics

Elke Theeuwes[1], Pieter Billen[1], Yoshi Marien[1], Christophe Vande Velde[1]
[1]Intelligence in Processes, Advanced Catalysts and Solvents (iPRACS), Faculty of Applied Engineering, University of Antwerp, Belgium

For decades value chains have been optimized to create functional materials, with a primary focus on performance. Gradually society has come to realisation that end-of-life of these materials must be considered throughout the value chain. There is a growing need for circular materials and waste conversion technologies, prompted by environmental concerns, need for securing resources and maintaining economic competitiveness towards materials from other global regions. Currently, the largest and easiest plastic waste streams (PE and PP) are being covered by scaling technologies, but there is still a huge potential for hard-to-recycle thermosets, like polyurethane, polyamides and vulcanized rubber.
We will present several industry cases to showcase hurdles and how to tackle them throughout the new circular value chain. Converting a linear value chain into a circular one, requires optimizing all steps and rethinking old go-to-solutions, during polymer development, article creation, waste collection, sorting, and depolymerisation processes.
Firstly, during the polymer development process, monomers and additives are selected to manufacture on-spec products. For example, the impact of pigments in polyurethane depolymerisation was investigated to provide recommendations towards new polymer designs. Secondly, polyamide polymers are used in a variety of materials, besides textiles, for instance in power tools and cars. This has an impact on the waste collecting and sorting. A thorough identification and separation of the polymeric nature of the waste streams, linked to an adequate depolymerisation step, can yield circular raw materials that can be plugged into making new polymers. Thirdly, technology assessment and development can aid in designing new processes, to obtain platform molecules. For example, using ozonolysis to convert end-of-life rubber into oxidised carbon black, levulinic and succinic acid. Finally, at each step the complexity can be quantified in terms of statistical entropy, resulting in a hands-on management decision making tool.

Acknowledgements to the financial support of Provincie Antwerpen (PA-Link project), and to the FWO (scholarships Yanou Fishel (file number 1S93022N) & Jonas Cassimon (file number 1S09725N).

CCS - D4 - O01

Mechanochemistry in batch and continuous - A transformative opportunity for sustainable pharmaceutical manufacturing: Case studies

Christos M. Chatzigiannis, Ruben Solorzano-Rodriguez, Corentin Bordier, Evelina Colacino
ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France

Although there have been efforts to reduce the environmental impact of active pharmaceutical ingredient (API) production, the use of organic solvents (responsible for 75% of energy used) is still a critical step in many processes. Solvent-free (or low solvent) synthesis by mechanochemistry is Safe and Sustainable by Design (SSbD) and offer an eco-friendly[1-3] and cost-effective pathway to green pharmaceuticals.[4] We report herein a comprehensive study for the total mechanochemical synthesis of a high-value immunomodulatory drug, also listed as essential medicine by the World Health Organisation (WHO). Moving beyond standard milling techniques, process scalability via Resonant Acoustic Mixing (RAM) and Twin-Screw Extrusion (TSE) was demonstrated, bridging the gap between technologies, by systematically mapping the transition from batch to continuous processing.

The multi-step mechanochemical synthetic sequence consisted in a one-pot cascade alkylation-intramolecular amidation reactions, followed by a metal-free reduction step under mild conditions, avoiding the use of gaseous hydrogen. The waste generated are non-toxic, and the by-product was converted in the desired target during the downstream process.

This multi-platform approach allowed us to de-risk the scale-up of rheologically complex intermediates, enabling a seamless translation from gram-scale protocols to continuous production with throughputs increased by orders of magnitude. This work illustrates a robust workflow for scaling mechanochemical processes, offering a concrete blueprint for the sustainable manufacturing of complex pharmaceuticals.

The authors acknowledge IMPACTIVE (Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients), the research project funded from the European Union's Horizon Europe research and innovation programme (European Health and Digital Executive Agency) under grant agreement No. 101057286. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or (European Health and Digital Executive Agency). Neither the European Union nor the granting authority can be held responsible for them.

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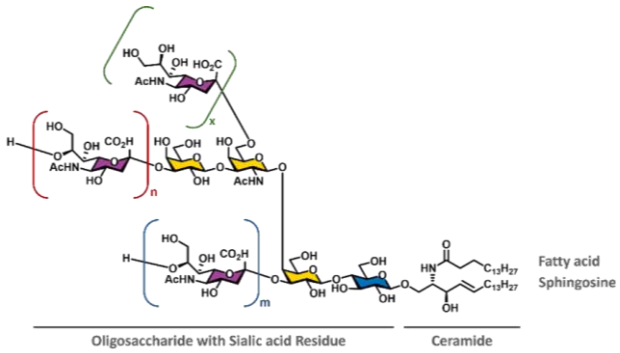
[4]IMPACTIVE (Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients), www.mechanochemistry.eu, and https://cordis.europa.eu/project/id/101057286

CCS - D4 - O03
Chemoenzymatic synthesis of gangliosdies

Chun-Cheng Lin, Hsin-Kai Tseng, Shu-Yen Chang
Dept. of Chemistry, National Tsing Hua University, Taiwan

In this study, we established a versatile and highly efficient enzymatic platform for the synthesis of a broad spectrum of natural ganglioside glycans by integrating sequential glycosyltransferase (GT) reactions with sugar-nucleotide regeneration or one-pot multienzyme (SNRS or SOPME) strategies. Using a simple Lac-β-O$(CH_2)_6N_3$ acceptor as a universal scaffold, we constructed a diverse library of ganglioside glycans. Importantly, bacterial α2,6-sialyltransferases (Pd2,6ST and Psp2,6ST) were found to regioselectively install α(2,6)-Neu5Ac onto internal GalNAc residues, providing a cost-effective and robust alternative to mammalian enzymes for the preparation of structurally defined sialylated glycans.
To further expand the scope of α2,6-sialylation, human ST6GalNAc5 (hST6GalNAc5) was recombinantly expressed in Expi293F™ cells at 32 °C, affording high enzyme yield and enhanced catalytic activity. Comprehensive kinetic and substrate-specificity analyses revealed a strong preference for Sia-α2,3-Gal and Gal-β1,3-GlcNAc/GalNAc motifs, while oligo-sialylated lacto-*N*-biose derivatives were also efficiently accepted. Coupling hST6GalNAc5 with SNRS enabled the high-yield synthesis of multiple complex sialylated glycans, including DSLNT, Lstb, GT1aα, and GQ1bα, and other structurally elaborate glycans, demonstrating its broad donor tolerance toward C5-modified CMP-sialic acids.
Notably, the scalable one-pot synthesis of DSLNT derivatives from lactose, reaching 340 mg, underscores the translational potential of this platform for producing bioactive human-milk-oligosaccharide-like glycans as nutritional additives. Collectively, this work establishes hST6GalNAc5-enabled chemoenzymatic synthesis as a powerful approach for accessing multisialylated glycoconjugates that were previously difficult to obtain, thereby advancing glycan-based immunological and therapeutic research.



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CCS - D4 - O04

Can proteins be fast and selectively cleaved under mild conditions without using proteases? A bimetallic Ce-MOF artificial nanozyme answers

Rongwei Gao[1], Evy Timmerman[2], Simon Devos[2], Francisco de Azambuja[1,*], and Tatjana N. Parac-Vogt[1,*]
[1]KU Leuven, Dept. of Chemistry, Belgium; [2]VIB Center for Medical Biotechnology, Belgium

The development of efficient and selective artificial proteases under mild conditions remains a key challenge in bioinorganic catalysis[1, 2]. Herein, we report a cerium–copper bimetallic metal–organic framework (Ce-MOF-818) capable of site-selective hydrolysis of myoglobin (Mb) under physiological conditions (pH 7.4, 25–60 °C)[3]. In contrast to pure Ce and Cu counterparts, which exhibit negligible or weak activity, Ce-MOF-818 demonstrates robust hydrolytic efficiency, affording 8 distinct fragments and with near-complete protein hydrolysis after 48h of incubation at 60℃ and pH 7.4. Mechanistic investigations support a cooperation between spatially proximate Cu and Ce nodes. Cu^{2+} facilitates substrate anchoring via coordination with histidine residues, while Lewis acid Ce^{4+} centers likely assist peptide cleavage by increasing peptide bond polarization. These findings highlight Ce-MOF-818 as a promising nanozyme platform that integrates substrate recognition and cleavage functions for potential applications in proteomics, biomolecule engineering, and diagnostics.

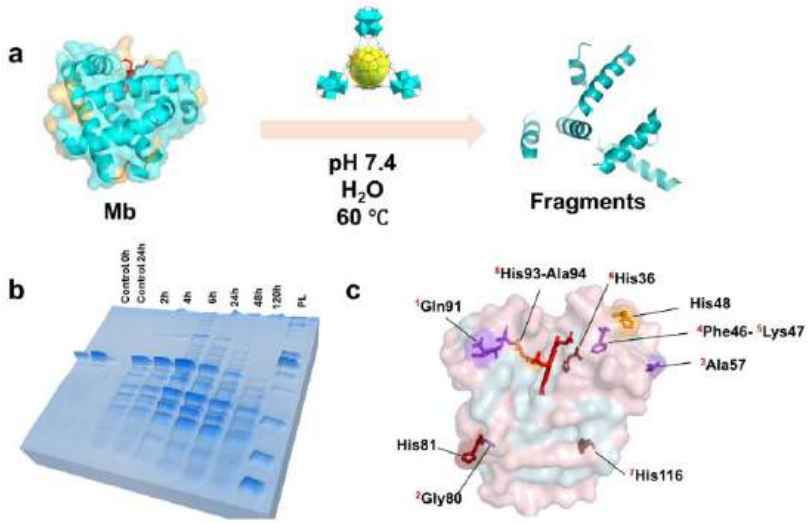

Fig. 1. a) Protease-like activity of Ce-MOF-818. b) Silver-stained SDS-PAGE analysis at different reaction times indicates that Ce-MOF-818 exhibits efficient protein cleavage activity. PL = protein ladder. c) Ribbon model of Mb shows cleavage sites are predominantly located near histidine-rich regions . Cleavage sites (purple), histidine residues (orange), and overlapping residues that are both cleavage sites and histidine (dark red).

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CCS - D4 - O05
Carbon nitride photocatalysis for additive-free vicinal halotrifluoromethylation of unactivated alkenes

Theodore Anthony Gazis[1], Gianvito Vilé[1]
[1]*Politecnico di Milano, Italy*

Vicinal halotrifluoromethylation of unactivated alkenes is a step-efficient route to trifluoromethylated building blocks that simultaneously introduces a halide handle for downstream derivatisation. Despite its synthetic value, visible-light halotrifluoromethylation remains dominated by homogeneous photoredox protocols that often require additives and limit catalyst recovery and reuse.[1,2] Here we report a sustainable, metal-free heterogeneous alternative based on carbon nitride photocatalysis. (**Figure 1**)
Using commercial triflyl chloride (CF_3SO_2Cl) as a bifunctional radical source, carbon nitride nanosheets enable additive-free halotrifluoromethylation, delivering β-CF3 alkyl halides in high yields. The nanosheet catalyst outperforms bulk carbon nitride, consistent with higher accessible surface area, and control experiments confirm that both irradiation and the photocatalyst are essential. The methodology accommodates electronically diverse styrenyl and allylic substrates, sterically demanding alkenes and phenolic natural-product derivatives without protection groups, with excellent chemoselectivity across pharmaceutical, agrochemical, and fragrance motifs. The approach also extends to other halide variants and related perfluoroalkylation. Photoluminescence quenching studies and radical-trapping experiments support a non-radical chain pathway in which triflyl chloride is the dominant quencher.
A key practical advantage of the heterogeneous platform is straightforward catalyst recycling by filtration, with no loss of activity over five runs. To overcome photon-transport limits that typically constrain batch heterogeneous photochemistry, we implement a packed-bed reactor. This enables, to our knowledge, the first continuous-flow vicinal halotrifluoromethylation and delivers an order-of-magnitude increase in productivity (mmol/h) relative to batch operation. (**Figure 2**)
Overall, carbon nitride provides a recyclable, additive-free platform for visible-light vicinal halotrifluoromethylation, pairing scope and efficiency with straightforward scalability.

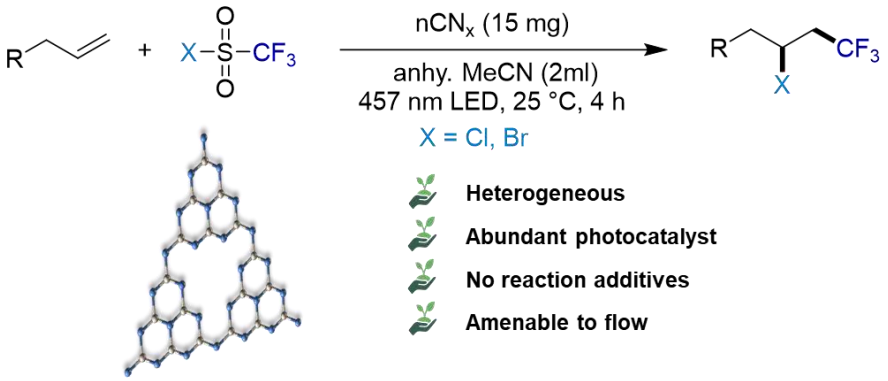

Fig. 1. Top: reaction scheme. Bottom: schematic depiction of carbon nitride.

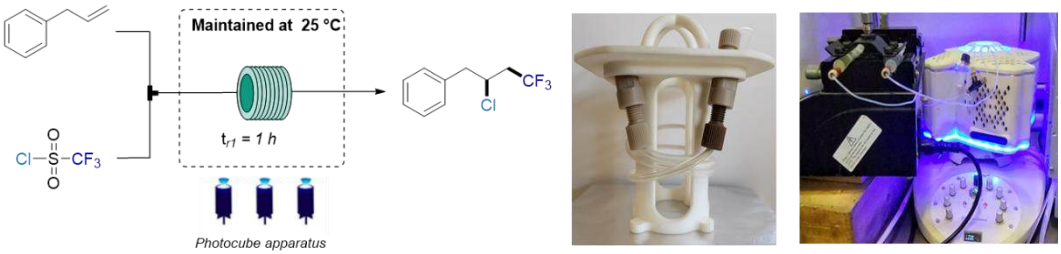

Fig. 2. Left: continuous-flow scheme. Right: pictures of packed-bed reactor and reactor system.

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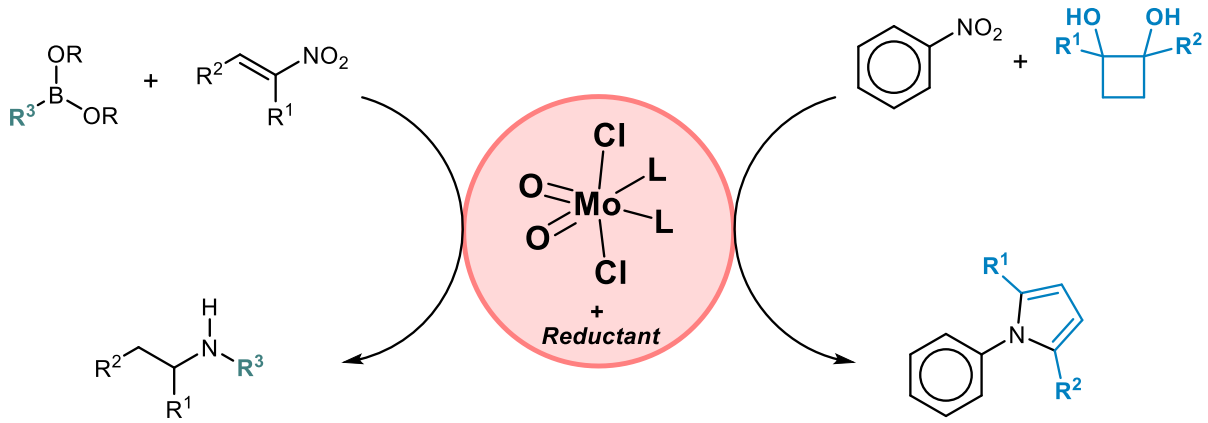
CCS - D4 - O06

Direct synthesis of secondary amines and *N*-based heterocycles from nitrocompounds under molybdenum catalysis

Samuel Suárez-Pantiga[1], Roberto Sanz[1]
[1]Depto de Química, Universidad de Burgos, Spain

Dioxomolybdenum complexes have been demonstrated to be effective catalysts in a plethora of deoxygenation reactions involving the cleavage of S–O, N–O, or even C–O bonds.[1] Among the various substrates explored in these transformations, nitroaromatic compounds have revealed as particularly versatile reactants, enabling access to a broad array of molecular scaffolds depending on the choice of the reducing agent,[2-3] while also facilitating C–N bond formation C–N bonds. In this sense, the use of 1,2-diols as reductants generates carbonyl by-products that are efficiently engaged in cyclization reactions.[1,2] An example of this reactivity is the direct synthesis of pyrroles from nitroaromatics in the presence of 1,2-butanediols and pinacol.[4] Additionally, the combination of nitroarenes with boronic acids as coupling partners, and phosphines as reductants, under dioxomolybdenum catalysis, enables the formation of diarylamines via reductive coupling reactions.[5] Similarly, nitroalkenes, when combined with a suitable reducing agent, can also undergo coupling reactions with boronic acids, providing straightforward access to a variety of secondary amines



Acknowledgements: The authors acknowledge financial support from Ministerio de Ciencia, Innovación y Universidades (PID2023-148198NB-C21/AEI/10.1039/501100011033), and Junta de Castilla y León and FEDER (BU028P23). S.S.-P. thanks Ministerio de Ciencia, Innovación y Universidades and “NextGenerationEU”/PRTR EU for a Ramón y Cajal contract (RYC2021-031533-I).

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CCS - D4 - O07
Mechanochemistry: A different path to selective hydrogenation

Maike Mayer[1], Lars Borchardt[1]
[1]Ruhr-University Bochum, Germany

Mechanochemistry is a growing field of chemistry, allowing direct processing of solids without the need for solvents. Reactions are facilitated by mechanical impact, commonly in ball mills. This is particularly interesting for catalytic reactions between gases and solids, as this approach avoids issues caused by gas solubility and diffusion; both solid and gas are in direct contact with the catalyst. We show that this process allows versatile hydrogenation reactions with notable selectivity. By electroplating the reaction vessel (Fig. 1a) with a nanolayer of various catalysts, we introduce an easily recyclable, highly active catalyst with competitive turnover numbers and frequencies. This allows hydrogenation of olefins, carbonyl- and nitro-groups, as well as dehalogenation at ambient temperature and low pressure. By adjusting milling conditions and catalyst choice, chemoselective transformations are achieved, such as nitro-group reduction and carbonyl reduction in presence of halogens (Fig 1b).[1] Additionally, modification of the nanolayer enables selective semi-hydrogenation of alkynes to alkenes. When pairing the palladium layer with simple organic nitrogen bases like pyridine as modifiers, alkynes like tolan are transformed to the *Z*-alkene selectively with 98% selectivity at 97% conversion (Fig. 1c). Operando surface-enhanced IR spectroscopy of the catalyst confirms rapid adsorption of pyridine, displacing alkene from the surface, avoiding further hydrogenation. Ball milling reduces the residence time of the substrate at the catalyst further increasing selectivity. The adsorption heat of the modifier on the palladium surface is found to be the key factor in selectivity. These results establish catalytic nanolayers coupled with organic ligands as a simple, effective, and lead-free approach to selective hydrogenation.

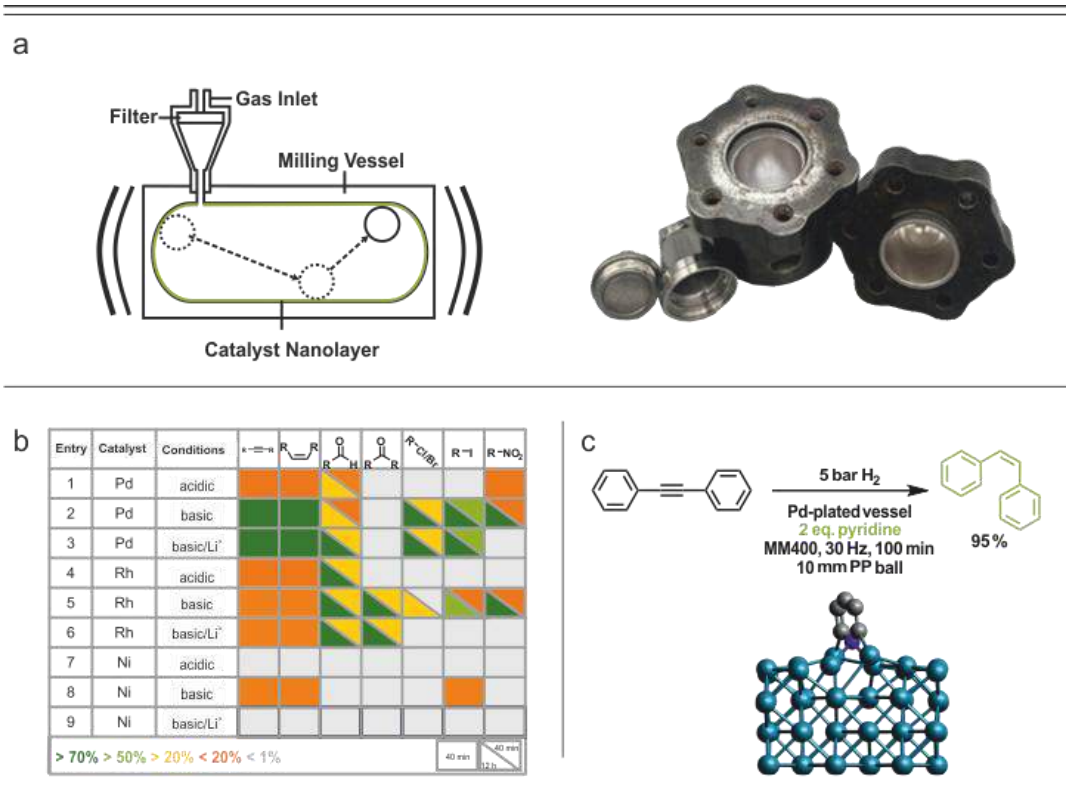

Fig. 2. a. Set-up for mechanochemical Hydrogenation. b. Chemoselective Hydrogenation of various functional groups. c. Selective Semi-Hydrogenation of Alkynes using poisoned palladium-surfaces.

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CCS - D4 - O08

Opportunities and challenges of in situ & ex situ electro-organic synthesis with H_2O at transition metal catalysts

Patrick Mollik[1], Tianyin Huang[1], Helena Pletsch[1], Dominik P. Halter[1,2]
[1]Technical University of Munich, Germany; [2]University of Antwerp, Belgium

Electro-organic synthesis with H_2O as a reagent, catalyzed by transition metal complexes and materials provides a powerful connection between renewable energy, sustainable reagents, and needs of the base-chemical value chain. Cathodic e-hydrogenation, anodic oxygen atom transfer (e-OAT) and hydrogen atom transfer reactions (e-HAT) are crucial reactions in this context. Developing such reactivity towards useful applications requires further innovation on both fundamental chemistry and process engineering. Specific challenges include control over product selectivity, first and foremost to prevent parasitic H_2 and O_2 evolution from the H_2O reagent in favor of controlled reaction with organic substrates.[1] Additionally, selectivity of target substrate conversion, exemplarily in semi-hydrogenation of alkynes, or alcohol oxidation to aldehydes instead of carboxylic acids remains complex.
The presented work will showcase different strategies to achieve such reaction control. Part one covers how oxidative addition of H_2O can be used as a mechanistic alternative to proton reduction, in order to generate active metal-hydride species without H_2 evolution even in alkaline conditions. Structure-function correlations of molecular iridium-pincer electrocatalysts are then used to tune reactivity and break traditional correlations between selectivity, kinetics, and thermodynamic driving force.[2] Spectro-electrochemistry and mechanistic studies are included to rationalize the findings and to derive future catalyst design guidelines. In a second part, ex situ electrosynthesis will be presented as a new method that uses energy storing electrocatalyst materials, to separate chemical and electrochemical steps of an electrocatalytic cycle in time and space.[3] This approach allows to synthesize previously inaccessible products with orthogonal selectivity to traditional electrolysis with substrates in the electrolyzer.

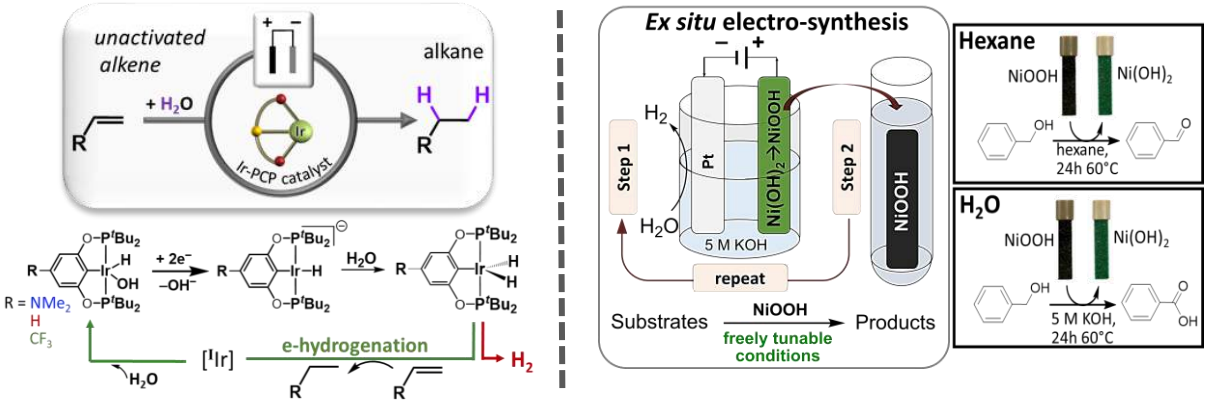

Fig. 1. *Left*: Electro-hydrogenation with Ir-pincer catalysts and H_2O, proceeding through highly reactive anionic Ir(I)-hydride species, characterized by mass spectrometry and low temperature NMR for the first time. *Right*: Overview scheme of the two-step ex situ electro-organic synthesis process that allows reactions at activated catalyst materials under different conditions than in the electrolyzer.

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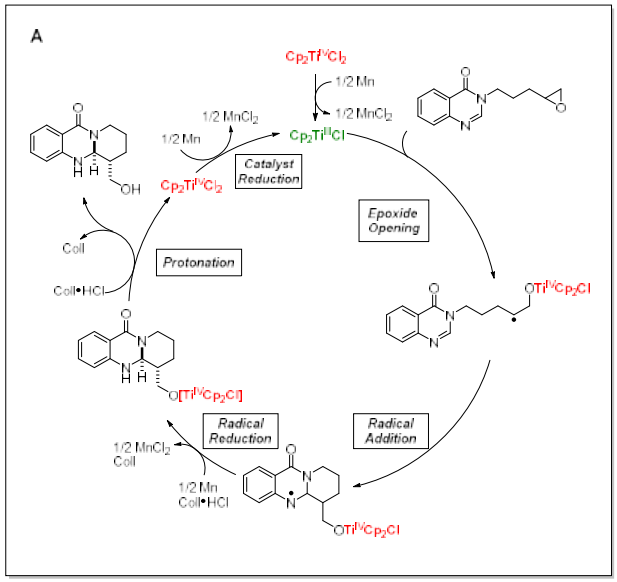
CCS - D4 – O09
Dihydroquinazolinones by titanocene catalyzed reductive radical addition to quinazolinones

Thomas Heinrichs[1], Konstantin Woitol[1], Andreas Gansäuer[1]*
[1]T. Heinrichs, K. Woitol, Prof. Dr. A. Gansäuer, Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Germany

In this study, we present a novel method for the synthesis of functionalized dihydroquinazolinones through an intramolecular radical addition to quinazolinones, catalyzed by titanocene. The mechanistic key issue is the reduction of the radical σ–complex formed after the addition of the epoxide-derived β–titanoxy radical. This reduction is unprecedented in titanocene-catalyzed radical arylations. The diastereoselectivity of product formation is high, and a number of functional groups are tolerated in the pharmaceutically relevant 6- and 7-positions of the dihydroquinazolinone products. If desired, these products can undergo oxidation to the corresponding quinazolinones with MnO_2.



CCS - D4 - O10
Upcycling potentially waste-derived Silicon into novel heterogeneous catalysts

Maria Teresa Tiberi[1], Giulia Brufani[2], Luigi Vaccaro[1]
[1]Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Italy; [2]Dept. of Civil, Energy, Environmental and Material Engineering (DICEAM), Università degli Studi Mediterranea di Reggio Calabria, Italy

In the catalytic sector, noble-metal catalysts supported on silica and activated carbon constitute a significant market segment. However, research efforts are increasingly directed toward the development of cost-effective supports derived from waste streams that are competitive with widely used and conventional material. Despite the quite long average lifetime of PV, estimated based on guaranteed performance,[1] their utilisation generates a significant amount of waste, raising both environmental and economic concerns for the global community. The global volume of End-of-Life modules is indeed projected to reach approximately 78 million tonnes by 2050[2]. That's why Silicon that accounts for more than 3.65 wt% of each module, can be regarded as high-value material with strong potential for urgent upcycling. In this context, end-of-life silicon finds applications in different files, including as anodes in lithium-ion batteries,[3,4] and CO_2 reduction[5], but the examples in catalysis are limited. We propose easily available, locally sourced, and potentially photovoltaic-waste-derived silicon-based heterogeneous support capable of retaining metallic nanoparticles as a promising alternative to conventional carbonaceous supports. The resulting catalysts were evaluated in benchmark reactions to explore their performances in obtaining high market potential molecules.

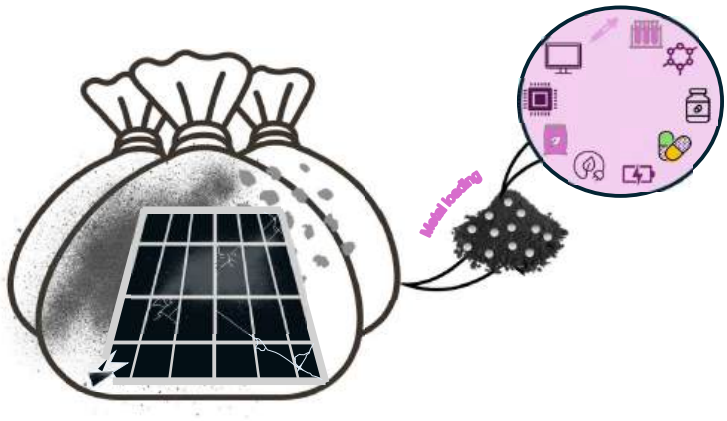


Fig. 1. graphical abstract

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CCS - D4 - O11
Precise regulation on the interfacial atomic structures of carbon-based hybrid materials

Zhihong Tian[1]*
[1]*Institute of Nano Sciences and Engineering, Henan University, China*

The practical applications of carbon-based hybrid materials in the fields of energy and environment are severely restricted by poor controllability of interfacial structures and thus low-efficiency charge transfer. To this end, the reporter has carried out systematic studies on the regulation of interface structures and charge transfer efficiencies of carbon-based hybrid materials, and developed the following strategies: (1) the confined pyrolysis was developed to precisely regulate the atomic arrangement of B/N heteroatoms at the interface of carbon-based hybrid materials, which can contribute to the revealing of relationship between the interface structures and electrochemical activities; (2) a new strategy of salt template-induced conjugated bonding of interfacial atoms was developed, benefiting the controllable construction of three-dimensional regular polar pore structures in carbon-based hybrid materials; (3) heterogeneous interfaces were well constructed through in-situ evolution of metal-based polymers, providing controllable interfacial bond strengths and valence states and thus improved charge transfer efficiency. Those studies could provide insight into the development of carbon-based hybrid materials for practical implements in electrocatalysis, energy storage, and environmental technologies.

[1]Wang, S.[†]; Zhou, S. J.[†]; Ma, Z. P.[†]; Gao, N. N.; Daiyan, R.; Leverett, J.; Shan, Y. H.; Zhu, X. F.; Zhao, Y. F.; Liu, Q.; Amal, R.; Lu, X.Y.; Liu, T. X.; Antonietti, M.; Chen, Y. G.; Zhang, Q. R.;* Tian, Z. H.* *Angew. Chem. Int. Ed.* **2025**, *64*, e202501896.
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CCS - D4 - O12

High-yield methane pyrolysis over hydrotalcite-derived Ni/Al_2O_3 in a fluidized bed reactor

Daan van Eck[1], David Reus[2], Mees Emond[1], Kay Buist[2], Petra de Jongh[1]

[1]Institute for Sustainable and Circular Chemistry, Utrecht University, The Netherlands; [2]Multi-scale Modelling of Multi-phase Flows, Eindhoven University of Technology, The Netherlands

Methane pyrolysis is an innovative H_2 production route without direct CO_x emission. Typically, Ni catalysts are used due to their high intrinsic CH_4 decomposition activity and co-production of a tunable nanostructured carbon product. The main challenge is their limited lifetime due to amorphous carbon buildup. Industrial application of Ni catalysts requires a combination of high activity and stability. Studies have so far reported high carbon yields and long lifetimes only when the carbon production rate was low.[1] Here, we report an effective Ni/Al_2O_3 catalyst derived from a hydrotalcite-like compound that was tested for methane pyrolysis in a fluidized-bed reactor under industrially relevant hydrodynamic conditions (GHSV = 640 000 $mL_n\ CH_4\ g_{cat}^{-1}\ h^{-1}$). The catalysts exhibited high initial reaction rates (20-45 $g_c\ g_{cat}^{-1}\ h^{-1}$) and reached carbon yields of >200 $g_c\ g_{Ni}^{-1}$ while being active for up to 8 hours. The highest carbon yield was obtained at 550 °C with an inlet feed of 80% CH_4 and 15% H_2 and is amongst the highest reported in a fluidized-bed reactor in literature so far.[2,3] The carbon product was characterized as carbon nanofibers with interesting properties ($d_{average}$ ≈ 30 nm, I_D/I_G = 1.6-1.8) and good thermal stability ($T_{decomposition}$ ≈ 580 °C in 20% O_2/Ar). A kinetic model that takes into account internal diffusion accurately predicted the initial reaction rate across different process conditions (R^2 = 0.9857). Furthermore, SEM analysis revealed the growth of immense carbon granules from 0.36 mm to more than 2 mm. We will discuss in detail what limits the final carbon yield and how it might be increased further.

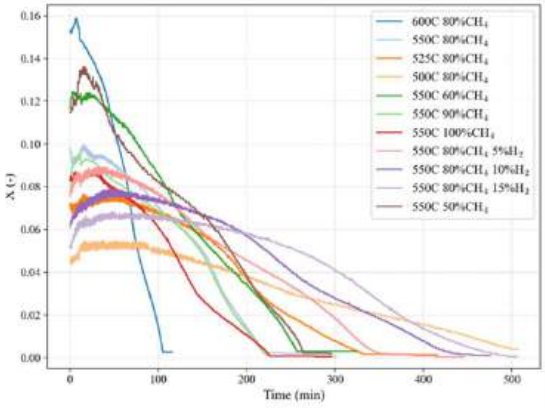

Figure 1. Methane conversion over time of Ni/Al_2O_3 under different operating conditions. Catalyst loading: 0.3 g., sieving fraction 300-420 um, GHSV = 640 000 $mL_n\ CH_4\ g_{cat}^{-1}\ h^{-1}$

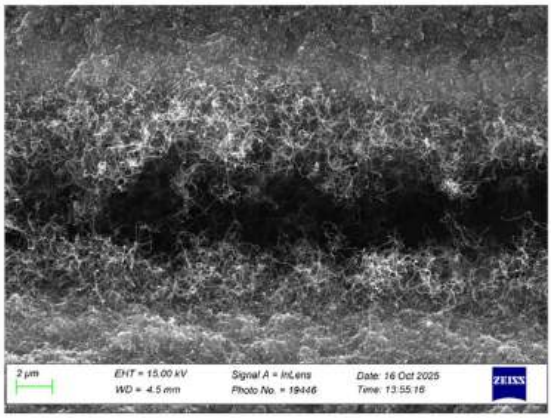

Figure 2. SEM image of a channel in the carbon granule post-catalysis, showing the formation of large amounts of carbon nanofibers.

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Energy, Environment & Sustainability (EES)

EES - D1 - O01

Supramolecular architectures for hydrogen generation at neutral pH conditions

Athira Ravi[1,2], Éadaoin Whelan[1], Gearóid Manning[1,3], Navaneetha Tokala[1,3], Claire Bradley[1,3], Karl Ackland[1,3], Matthew Murlidhar[1], Nianyong Zhu[1], Wolfgang Schmitt[1,2,3 *]

[1]School of Chemistry, Trinity College Dublin, IR; [2]Research Ireland Centre for Pharmaceuticals (SSPC), University of Limerick, IE; [3]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) & AMBER, Trinity College Dublin, IE

Supramolecular coordination cages provide discrete 3D cavities that facilitate site-isolated catalysis and molecular recognition.[1] Current design strategies prioritize tailorable topologies to exploit space-restricted effects, particularly for the electrochemical hydrogen evolution reaction (HER), where confined microenvironments stabilize intermediates to enhance catalytic performance.[2] A supramolecular strategy for constructing free-standing,{Cu_2}-based hydrogen evolution reaction (HER) electrodes with exceptional catalytic performance under near-neutral conditions is investigated. The approach employs electron-rich thienothiophene (H_2CPTT) carboxylate ligands that assemble with Cu(II) ions into redox-active {Cu_2} paddlewheel units, forming a porous metal-organic polyhedron (MOP), [$Cu_{18}(CPTT)_{18}(H_2O)_{18}$], with rare hendecahedral topology. Remarkably, the species can be grown directly *in-situ* on copper substrates, such as microporous foams, either through bulk solvothermal routes or rapid (<5 min) cathodic electrodeposition, yielding robust, catalytically accessible, and electronically integrated electrodes. The experiments highlight the effectiveness of leveraging porous, supramolecularly defined cavities in MOPs as a general design concept for catalytic enhancement.[3] Methyl viologen incorporation enhances charge-transfer highlighting the promise of biomimetic host-guest architectures for improved H_2O reduction. Electrochemical studies reveal outstanding HER activity, with a current density of –340 mA cm^{-2} at –0.65 V *vs*. RHE, an overpotential of –0.115 V at -10 $mAcm^{-2}$, and a Tafel slope of 69 $mVdec^{-1}$.This supramolecular assembly method is easily generalizable to other carboxylate ligands and metal centres, offering a potentially scalable and synthetically accessible route to high-performance molecular HER electrocatalysts, and a promising platform for next-generation molecule-based H_2 production technologies.

Research funding from Research Ireland, the European Research Council and the European Innovation Council is acknowledged.

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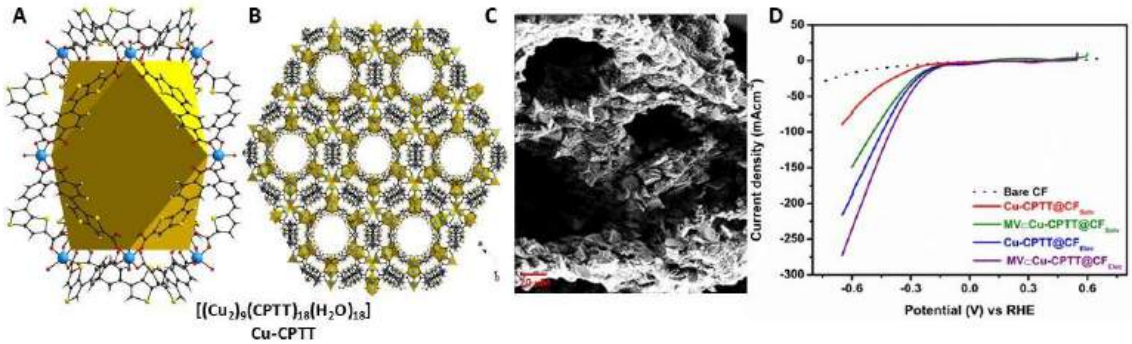

Fig. 1. A. Molecular structure of Cu-CPTT highlighting hendecahedral topology of Cu-CPTT with the centres of the {Cu_2} units defined as vertices, **B**. Supramolecular packing of molecular entities of Cu-CPTT with view in the direction of the crystallographic *c*-axis, **C**. FESEM image of Cu-CPTT grown on copper foam, **D**. Linear sweep voltammograms (LSV) demonstrating the influence of MV incorporation for respective electrodes.

EES - D1 - O02
Assembly-driven switching of a POM–carbon nanotube catalyst for acid water splitting

María Giménez López[1]*, Eugenia P. Quirós-Díez[1], Melanie Guillén-Soler[1]
[1]Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Universidade de Santiago de Compostela, ES

Efficient, durable electrocatalysts that operate under strongly acidic conditions remain a key bottleneck for scalable green hydrogen technologies, where state-of-the-art performance still relies heavily on scarce noble metals.[1,2] Here, an earth-abundant vanadium polyoxometalate (POM) platform is presented in which nanoassembly—rather than chemical modification—controls reactivity, enabling a single molecular cluster system to access two distinct catalytic outcomes in 1 M H_2SO_4. The decavanadate-based material $Na_4H_2O_{12}(CH_2OH)_3CNH_3)_2V_{10}O_{28}{\cdot}4H_2O$ integrates "non-innocent" Na^+ and TRIS-derived counter-cations whose functions are dictated by how the POM interfaces with carbon nanotubes (CNT).[3]
A simple physical mixture with CNT yields outstanding oxygen evolution activity at acid pH, reaching an overpotential of 0.34 V at 10 mA cm^{-2} with 80% Faradaic efficiency, outperforming IrO_2 benchmarks under identical conditions. In sharp contrast, directed assembly of the same molecular building blocks on CNT surfaces unlocks the TRIS triol functionality, generating a highly efficient hydrogen evolution catalyst with an onset potential of 0.07 V and 94% Faradaic efficiency, approaching Pt/C. In-operando confocal microscopy and theory reveal that crystal-interaction control and microenvironment engineering orchestrate this switching: OER proceeds through an alcohol oxidation reaction–mediated pathway, while HER benefits from TRIS acting as a proton-sponge that concentrates protons near the POM surface. These results establish controlled nanoassembly as a general strategy to program bifunctionality into molecular electrocatalysts for robust acid-driven water splitting.

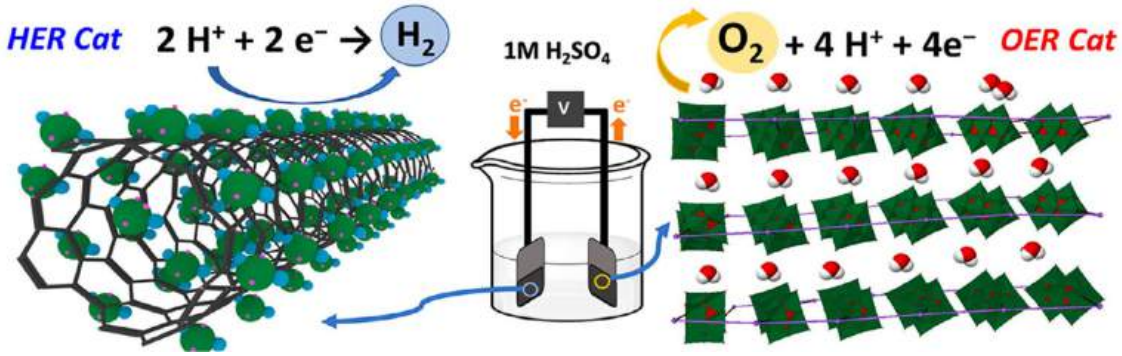

Fig. 1. Bifunctional behavior toward water splitting under strong acid conditions (1m H_2SO_4 previously degassed) of a vanadium POM-based carbon hybrid catalyst incorporating non-innocent cations depending on its assembly with carbon nanotubes (CNT).

This work has received financial support from the Ministry of Science and Innovation of Spain (Projects PID2021-127341OB-I00, PID2024-162420OB-I00) and Xunta de Galicia (for the Oportunius Research Professor Program.

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EES - D1 - O03

Laser-assisted synthesis of high entropy oxide-based freestanding electrode for electrochemical water splitting in alkaline conditions

Haider Ali[1], Sobia Dilpazir[1], Abuzar Khan[1]
[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum & Minerals, SA

The development of cost-effective, earth-abundant electrocatalysts for hydrogen evolution reaction (HER) remains critical for large-scale electrochemical water splitting applications. The conventional Ni-based electrodes in alkaline systems are cost-effective but suffers from relatively high overpotentials[1]. Recently, high entropy materials emerged as a stable and efficient electrocatalyst with comparable overpotential to platinum group metals. However, their synthesis techniques rely on energy and chemical intensive routes such as mechanochemical, co-precipitation and solid-state methods[2,3]. Moreover, immobilization of the electrocatalyst using a binding agent creates additional resistance to charge transfer. Therefore, a facile and cost-effective synthesis technique is needed for the development of freestanding high entropy material-based electrode.

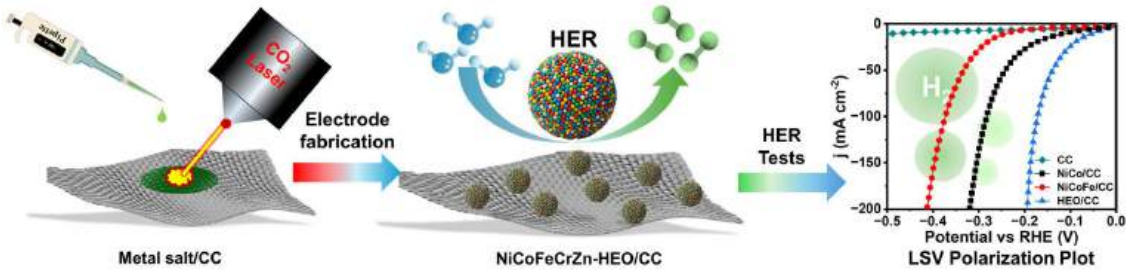

Fig. 1. Schematic illustration of the HEO-electrode fabrication and electrochemical tests.

This study presents a novel direct laser-assisted synthesis approach for fabrication of high entropy oxide (HEO)-based electrode. HEO consisting of five different metals comprising Ni, Co, Fe, Cr, and Zn was synthesized by drop-casting metal nitrate salts over a carbon cloth (CC) substrate followed by laser annealing. The localized laser irradiation instantly decomposed precursor metal nitrates, forming a well-adhered catalytic layer without binders. The prepared HEO was characterized by a range of physicochemical characterization techniques namely X-ray diffraction, electron microscopy and X-ray photoelectron spectroscopy. The HEO-modified carbon cloth electrode was tested in a 3-electrode assembly in alkaline conditions for hydrogen evolution reaction. The HEO-loading over the carbon substrate was optimized and the electrochemical tests were compared with oxide of NiCo and NiCoFe. Among the tested electrode, the HEO-based electrode achieved the lowest overpotential of 52 mV at 10 mA cm^{-2} with a Tafel slope of 125 mV dec^{-1}. Crucially, it exhibited a remarkable operational stability, maintaining activity for over 14 days at 100 mA cm^{-2}. Therefore, this work validates a facile, binder-free route to high-performance, durable HEO electrodes, presenting a significant step toward industrially relevant electrocatalyst fabrication for green hydrogen.

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EES - D1 - O04
Surface modified Nafion membrane for improved microbial fuel cell application

Priya Mukherjee[1], Fabian Fischer[1]
[1]Institute of Life Sciences, HES-SO Valais, University of Applied Sciences Western Switzerland, CH

The ever-increasing global population and urbanization have posed the challenge of enhanced energy requirements with the focus on renewable sources. The microbial fuel cell (MFC) is one such renewable technology that can generate energy from wastewater along with wastewater treatment. However, this novel technology depends on membrane for substrate separation and proton conductivity. Nafion membranes are the most widely used membrane in MFC applications. However, they are limited in their performance by allowing the passage of other cations present in wastewater along with protons[1]. Furthermore, they also allow the passage of oxygen and substate through their structure[2], leading to reduced power performance. In addition, they are susceptible to biofouling during long operations[3] and hence need improvement. The current study explores the effect of modifying the Nafion membrane with a conductive bio-inspired polymer polydopamine (PDA) with varying concentrations (PDA-1, PDA-2 and PDA-3) shown in Fig A and examining their performance for MFC applications. It was observed that the modified membrane had better hydrophilicity and proton conductivity compared to the unmodified Nafion membrane shown in Fig B. A maximum power density of 0.016 mW/cm^2 was achieved with the modified Nafion membrane which was around 2.3 times higher than the unmodified Nafion membrane.

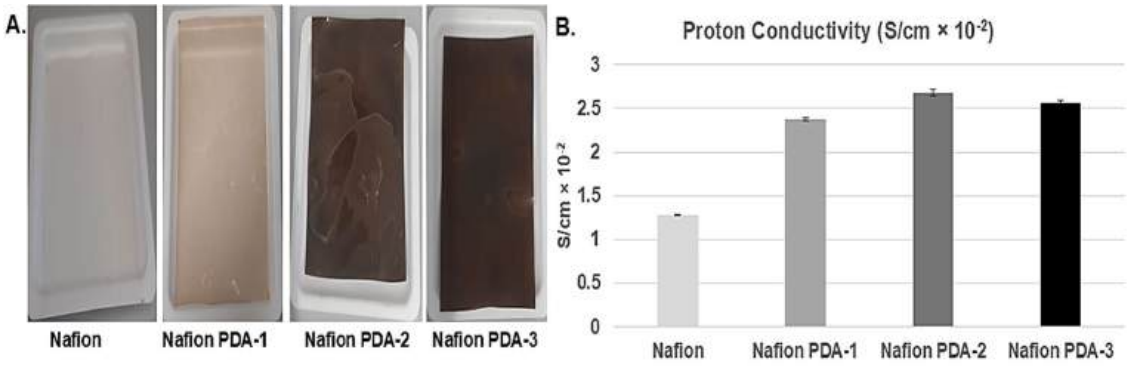

Fig. A. Modified Nafion membranes and B. their proton conductivity.

This work was financed by Swiss National Science Foundation (SNF, grant number 218849) and Slovenian Agency for Research and Innovation (grant number J2-50086) and program group P2-0118 Textile Chemistry and Advanced Textile Materials.

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EES - D1 - O05
Impact of stack architecture on stability and lifetime of CO_2-to-CO three chamber flow electrolyzers

Giovanni Di Berardino[1], Yu Zhang[1], Shankar Ram Ramakrishnan[1], Balamurugan Devadas[1], Nick Daems[1], Tom Breugelmans[1]
[1]ELCAT group, University of Antwerp, BE

The electrochemical reduction of CO_2 (CO_2RR) to CO in three chambers flow cells is a highly attractive technology for industrial carbon utilization, yet its large-scale deployment is strongly constrained by directly single cell scale-up and operating in high current density.[1] Cells stacking is an alternative strategy to increase throughput and reduce capital costs for high volume CO production. Appropriate stack architectures can influence the local environment and most importantly influence electrode degradation: such as electrode flooding, uneven reactant distribution, membrane dehydration, and local hot spots, all exacerbated under industrially relevant current densities and continuous operation.[2,3]
Here, we examine two representative modular stack designs for CO_2-to-CO flow-cell electrolyzers (100 cm² electrodes), focusing on stability-oriented strategies. The first configuration features a shared gas chamber supplying CO_2 to two opposing gas diffusion electrodes, combined with electrolyte streams arranged in a compact symmetric 1–2–3–2–1 configuration, where 1 is the anolyte chamber, 2 the catholyte chamber, 3 the gas chamber (Figure1a). While the second configuration uses fully modular stack design based on repeated 1–2–3 units (Figure1b).
Overall, this comparative analysis highlights the fundamental trade-off between individual cell control-oriented stacking and CapEx-driven compact stacking strategies. While modular designs favor stability and operability, highly compacted stacks (characterized by fewer compartments, higher product concentration, and enhanced single-pass conversion) offer substantial potential for system simplification and cost reduction. These results provide design-level insights to guide the development of stable and economically viable industrial CO_2 electrolyzer stacks.

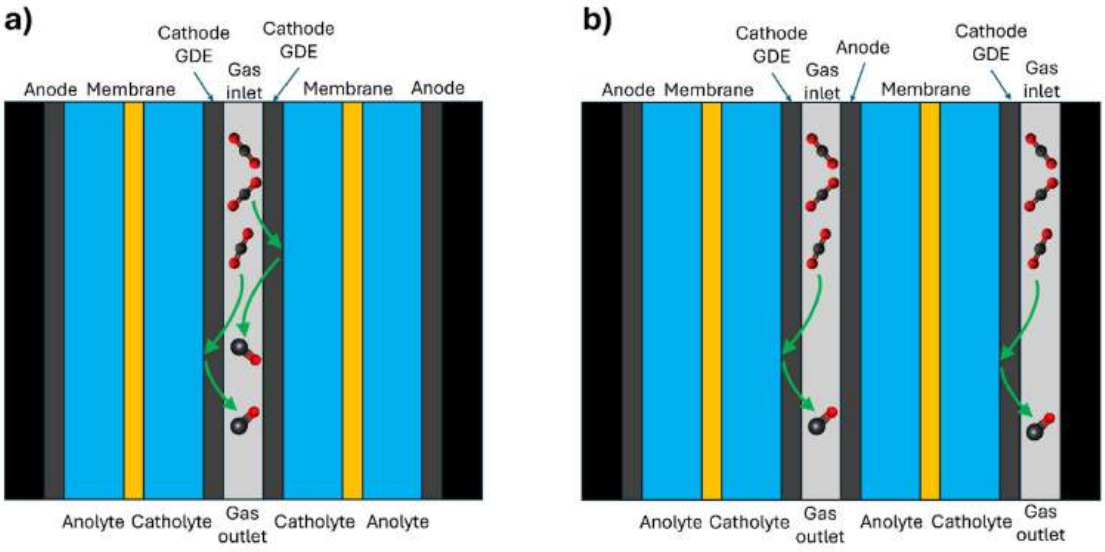

Fig. 1. Schematic representation of the two CO2-to-CO stacking strategies investigated in this work: (a) the compact architecture with only one gas chamber; and (b) the fully modular stacking design.

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EES - D1 - O06

Design and performance rationalization of blue-emitting copper(I) complexes bearing pyridyl-pyrazole ligands for light-emitting electrochemical cells

Chiara Reviglio[1], Luca M. Cavinato[1,2], Emanuele Priola[1], Sophia Lipinski[2], Youssef Atoini[2], Chiara Rosso[1], Claudia Barolo[1,3,4], Claudio Garino[1], Rubén D. Costa[2]

[1]Dept. of Chemistry, Università degli Studi di Torino, IT; [2]Chair of Biogenic Functional Materials, Technical University of Munich, DE; [3]Instm Reference Centre, IT; [4]ICxT Interdepartmental Centre, Università degli Studi di Torino, IT

Stable and efficient blue-emitting light-emitting electrochemical cells (LECs) remain one of the most persistent challenges in copper-based electroluminescent technologies, due to fast emitter degradation, unforeseen solid-state red-shifts, and aggregation-induced quenching.[1,2] Here, we report a systematic molecular-to-device study on a new family of heteroleptic tetrahedral copper(I) complexes of general formula [Cu(N^N)(P^P)]$^+$, specifically engineered to address these limitations through controlled steric and electronic tuning.

Following our previous work unlocking the first blue Cu(I)-LECs,[3] six novel pyridyl–pyrazole diimine ligands (N^N), functionalized with electron-donating and electron-withdrawing substituents, have been combined with xantphos (P^P) to afford highly emissive Cu(I) complexes all exhibiting thermally activated delayed fluorescence (TADF). The emitters display blue-to-cyan photoluminescence spanning 473–511 nm, solid-state photoluminescence quantum yields up to 71%, and short room temperature excited-state lifetimes down to 21 µs. Electrochemical studies reveal *quasi*-reversible redox behaviour, supporting their suitability for LECs application. Importantly, we confirmed that conventional single-parameter design rules fail to rationalize performance trends across solution, powder, and thin-film states.[4] To overcome this, a multivariate statistical analysis was applied, correlating structural descriptors (bite angles, Cu–N/Cu–O distances, torsional distortion), electronic parameters, and ligand polarity with photophysical and electroluminescent outputs. Crucially, it reveals that the key parameters governing photoluminescence quantum yield and device efficiency are distinct, as are those controlling emission maxima in powder versus thin films and the electroluminescence colour coordinates—providing definitive evidence of the intrinsic complexity of LEC performance rationalization.

LECs fabricated with these emitters achieve blue-green electroluminescence with luminance up to 230 cd m^{-2} and current efficiencies up to *ca.* 1 cd A^{-1} upon ionic optimization—among the best performances reported for pristine Cu(I)-based blue LECs. Overall, this work establishes a robust design framework for high-energy copper emitters and highlights multivariate analysis as a powerful tool to accelerate the development of sustainable, rare-metal-free lighting technologies.

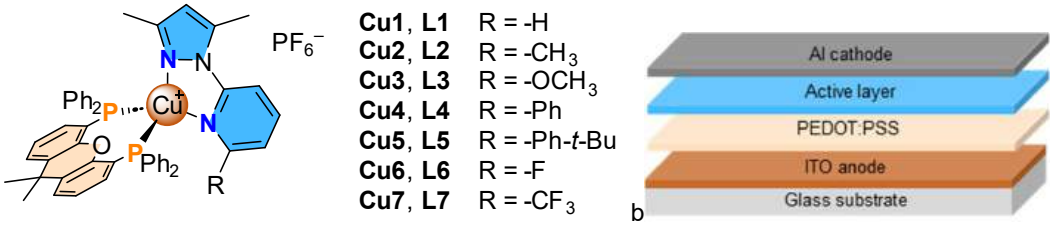

Fig. 2. a) Chemical structures of the copper(I) complexes **Cu1**–**Cu7**. b) Scheme of device architecture.

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EES - D1 - O07
CuO-based ionanofluids as advanced working fluids for high-efficiency solar collectors

Jesús León-García[1], José Javier Delgado-Marín[1], Imane Moulefera[1], Ignacio Carnerero[1], Mercedes G. Montalbán[1], Gloria Víllora[1°]
[1]Chemical Engineering Dept., Faculty of Chemistry, CEIR Campus Mare Nostrum (CMN), University of Murcia, ES

In this work, we present a detailed investigation of ionanofluids formulated with the ionic liquid [Emim][Ac] and copper oxide (CuO) nanoparticles, focusing on their stability, thermophysical properties, and performance as thermal fluids in a pilot-scale solar collector.. Among the tested formulations, the ionanofluid containing 0.5 wt% CuO proved to be the most promising, successfully combining adequate colloidal stability with significant enhancements in thermal conductivity and heat capacity compared with the pure ionic liquid. These improvements directly influence the collector's thermal behavior, particularly under low flow conditions (Figure 1), where longer residence times allow a more efficient utilization of the absorbed heat.
During the experimental tests, the CuO-based ionanofluid outperformed both water and the base ionic liquid, achieving the highest temperature increase and a markedly superior exergy efficiency. Under identical flow conditions, the ionanofluid exhibited an average exergy efficiency of 37.8%, whereas water reached only 24.8%, demonstrating a more effective conversion of the available solar energy into useful work. This enhancement is attributed to the combined effect of increased heat capacity and the reduction of thermal irreversibilities within the collector.
Based on the experimental findings, a series of advanced simulations was developed using specialized software [1], enabling the prediction of thermodynamic behavior under various operating scenarios for different ionanofluids. These simulations provide a valuable tool for preliminary optimization operating parameters and guiding the design of future experimental procedures.
The preliminary results obtained in this study are highly encouraging and indicate that metal oxide-based ionanofluids may effectively enhance the exergy efficiency of solar thermal collectors. Their improved thermophysical properties and superior thermodynamic performance reinforce their potential as advanced working fluids for next-generation solar thermal technologies.

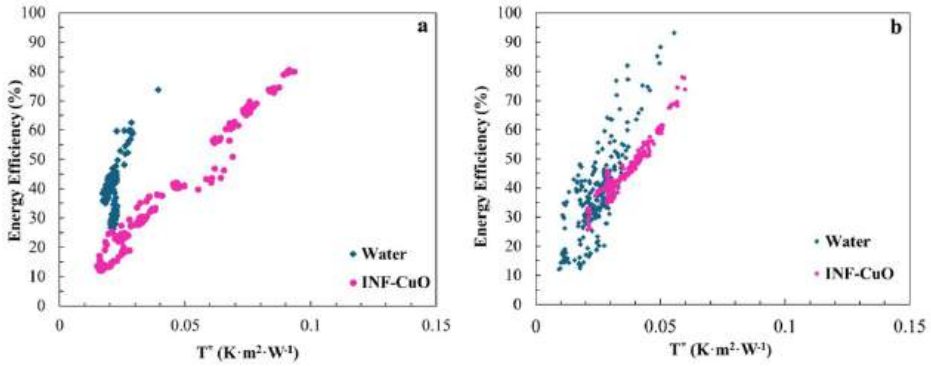

Fig. 3. Thermal energy efficiency of the FPSC at flow rate of; a) 6.12 L/h and b) 12.40 L/h.

Funding: This work is part of the following research projects: Ref. PID2023-150761OB-C21 funded by MICIU/AEI/10.13039/501100011033 and by FEDER, UE and Ref. 22129-PI-22 funded by the research support program of the Seneca Foundation of Science and Technology of Murcia, Spain. J.J. Delgado-Marín acknowledges support from the *Juan de la Cierva* contract (Ref. JDC2023-052774-I) funded by MICIU/AEI /10.13039/501100011033 and the FSE+.

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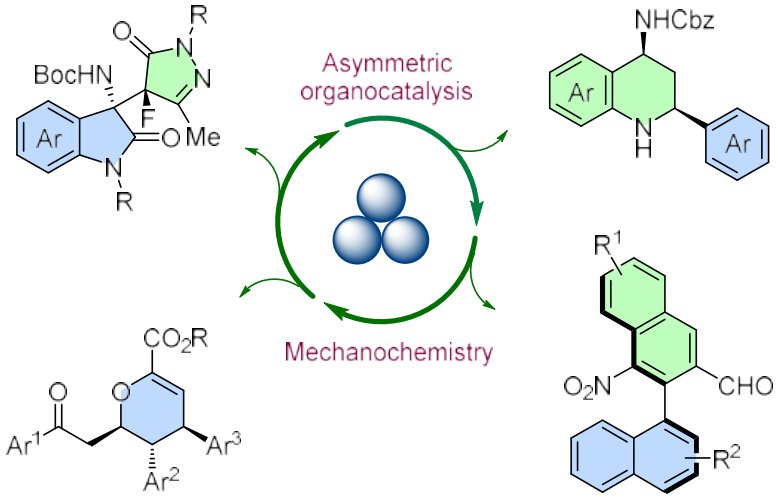
EES - D1 - O08
Making asymmetric organocatalysis greener and more efficient through ball-milling

Radovan Šebesta[1]
[1]*Comenius University Bratislava, Faculty of Natural Sciences, Dept. of Organic Chemistry, SK*

Asymmetric organocatalysis, as one of the pillars of asymmetric catalysis, is an indispensable tool for the synthesis of numerous chiral compounds. Merging asymmetric organocatalysis with mechanochemistry can further enhance the methodology's sustainability and efficiency.[1] Our recent work on mechanochemical organocatalytic domino Mannich reaction with fluorination shows that highly enantioenriched oxindolyl fluoropyrazolone products can be made in high yield and in short reaction times.[2] Formal organocatalytic cycloadditions under ball-milling conditions yield various chiral pyranes,[3] and tetrahydroquinolines.[4] Furthermore, we have shown the first example of a mechanochemical atroposelective transformation leading to axially chiral biaryls.[5] All these transformations benefit from liquid-assisted grinding, where the proper choice of liquid additive was key to achieving high yields and enantioselectivities. Moreover, minimization of bulk solvent use under mechanochemical conditions leads to a significant reduction in mass intensity.



Scheme 1. Asymmetric organocatalytic transformations enhanced by mechanochemistry.

This work was supported by the Slovak Grant Agency VEGA, grant no. VEGA 1/0445/24.

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EES - D1 - O09
The employment of mechanochemistry for the synthesis of thioureas and guanidines

Davor Margetić[1], Antonija Karakaš[1]
[1]*Laboratory for Physical Organic Chemistry, Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, HR*

Guanidines are very interesting molecules with remarkable physicochemical properties. In particular, high basicity (superbasicity) and the ability to form hydrogen bonds make guanidines suitable for various applications, such as organic catalysts and functionalities in anionic sensors. Various guanidine derivatives are found in nature and explored synthetically, and diverse synthetic routes and reagents were employed. Mechanochemistry has been recognised as a sustainable, solvent-free alternative to conventional organic solution-based synthesis.[1,2] The method offers several benefits, such as eliminating solvents, reducing chemical use, simplifying experimental procedures, and shortening reaction times, which are reflected in green chemistry metrics. Here, the explorative work on the mechanosynthesis of thioureas and guanidines from aromatic amines will be presented.

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EES - D1 - O10

Advances in sulphide mechanochemistry: From metal extraction to energy materials and anticancer drugs

Peter Baláž[1], Matej Baláž[1]
[1]Institute of Geotechnics, Slovak Academy of Sciences, SK

An important role of mechanochemistry[1] as an emerging alternative to solution-based chemistry in the synthesis and mechanical activation of sulphides is stressed out in this contribution. Selected results from science and technology applied in chemical engineering, materials science and medicine are illustrated. The golden thread in these activities is the mechanochemical treatment using high-energy mills in three selected modes (I-III). Knowledge obtained from the treatment of sulphides to extract metals (I)[2] is expanded to synthesis and application of energy materials (II)[2]. Non-traditional use of arsenic sulphides in cancer treatment is also illustrated (III). All the mentioned applications represent contribution to the common goal of mechanochemists: to prepare new materials with the desired properties in a reproducible way in easy-operating, environmentally friendly, green, sustainable and scalable manner and essentially waste-free conditions[4].

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-24-0353 and by the Slovak Grant Agency VEGA (2/0039/26).

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EES - D1 - O11

Mechanochemical approach for greener and effective recycling of platinum group metals from spent automotive catalysts

Zara Cherkezova-Zheleva[1], Daniela Paneva[1], Anna Vasileva[1], Kaloyan Ivanov[1], Anastasia Maria Moschovi[2], Iakovos Yakoumis[2]

[1]Institute of Catalysis, Bulgarian Academy of Sciences, BG; [2]MONOLITHOS Catalysts and Recycling Ltd, GR

Sustainable recycling of Platinum Group Metals (PGMs) from spent automotive catalysts represents both a challenge and possibility to address their increasing demand and limited supply. Conventional methods are effective but energy intensive, consume hazardous chemicals, and have significant environmental impact. Mechanochemistry is a promising green alternative, enabling induction of chemical reactions and activation of complex solid-state matrices under ambient conditions.

The study presents the benefits of using mechanochemical approach for treatment of spent catalytic converters toward sustainable, ecologically friendly and efficient extraction of PGMs. The parameters of applied mechanical energy are varied using different milling conditions (container/balls material, milling speed, ball-to-powder weight ratio and process duration), thus inducing cascade processes and structural disorder, lattice defects, and generation of nanosized domains. The obtained samples were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and Electron microscopy (SEM/EDS and TEM). The results indicate formation of amorphous phases and fresh reactive surfaces that enhance the dispersion and chemical availability of PGMs, improving metal accessibility and leaching efficiency.

According to Life Cycle Analysis, integration of mechanochemistry into recycling protocol demonstrates multiple advantages by reducing the use of aggressive reagents, energy requirements, processing complexity/steps, environmental footprint. Additionally, mechanochemical activation allows preparation of nano-dimensional precursors for synthesis of highly active and selective catalytic materials by reusing of as-recycled metals. Thus, mechanochemical treatment is not only an efficient recovery route but also a direct pathway toward the preparation of advanced materials in line with circular economy principles.

Acknowledgements: The authors gratefully acknowledge the support of project H2020-MSCA-RISE-2020 101007669: Chemistry of Platinum Group Metals, CHemPGM. Research equipment of the project № BG16RFPR002-1.014-0006 "National Centre of Excellence Mechatronics and Clean Technologies" was used for experimental work financially supported by European Regional Development Fund under "Research Innovation and Digitization for Smart Transformation" program 2021–2027.

EES - D1 - O12
Mechanochemistry as a sustainable tool for (de)racemization of biaryl atropisomers

Leon Poljanić[1], Tom Leyssens[1]
[1]*Université Catholique du Louvain, BE*

Atropisomerism is a form of axial chirality arising from hindered bond rotation.[1] Unlike stereocenter-containing compounds, often racemizing through bond breaking and formation, atropisomers racemize via bond rotation. Biaryl systems such as 1,1'-bi-2-naphthol (BINOL) and its derivatives have attracted significant interest due to their use as chiral catalysts and ligands in asymmetric synthesis.[2] Asymmetric synthesis is typically solution-based, requiring large quantities of solvent. With the current societal shift towards greener and more sustainable chemistry, mechanochemistry is gaining momentum as one of the solutions to this challenge.[3] However, mechanical energy can potentially induce changes in stereochemistry. We therefore investigated the stereochemical integrity of biaryl atropisomers under mechanochemical conditions typically used for asymmetric synthesis. We explored a variety of biaryl substrates, racemization catalysts, bases, presence of additives and liquid during grinding, and different reaction times. Under various conditions, biaryl atropisomers were found to undergo degradation, which can be attributed to several mechanistic pathways. The most prominent are racemization, oligomerization, and side product formation via intermolecular ring closure, including C-O and C-C bond formation. Moreover, we found that combining metal chlorides as racemization catalysts with different bases promotes degradation almost exclusively through racemization, leading to loss of enantiopurity without compromising catalytic activity. In contrast, oxidative pathways decrease catalytic activity, without affecting product enantiopurity. These findings highlight the interplay between enantiopurity and catalytic activity in ball milling, emphasizing the need for deeper investigation across a broader substrate scope and the mechanistic pathways behind these reactions.

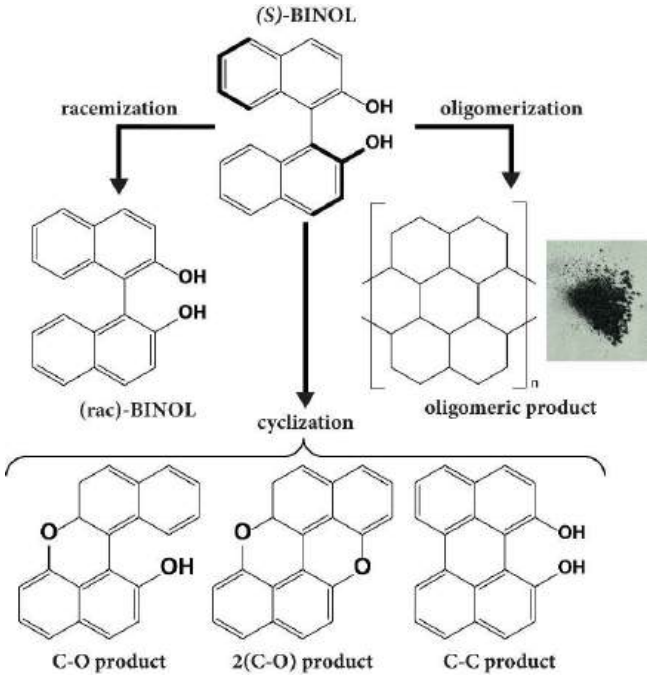

Fig. 1. *Possible mechanochemical degradation pathways of (S)-BINOL under ball milling conditions.*

L. Poljanic is funded by the FRIA doctoral grant.

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EES - D1 - O13
Chemical insights into triboelectric charging of polymers and organic powders

Bilge Baytekin[1], Niloofar Kamyar[1], Mahnam Ebadi[1], H. Tarik Baytekin[2], Erol Yildirim[2]
[1]Bilkent University, TR; [2]Middle East Technical University, TR

Insulating materials readily acquire electrostatic charge through contact, and the slow relaxation of these charges poses persistent challenges in industrial processes. Common consequences include material adhesion, flow disruption, agglomeration, and particle segregation, while uncontrolled charge discharge may lead to hazardous events such as fires or explosions, resulting in millions of dollars in annual losses. Addressing these issues requires a deeper mechanistic understanding of triboelectric charge generation and decay. Chemical insight into these two events can help address the challenges mentioned.
But *why the polymer and organic molecular compound powders*?
We focus on triboelectrification of organic bulk polymers and molecular powder compounds because these materials constitute a major class of insulators widely encountered in industrial applications. All branches of industry, i.e., pharma, air and space, textiles, food, and plastics, suffer from the aforementioned detrimental effects of tribocharging. Although triboelectrification in these materials has been studied extensively, existing knowledge is largely based on empirical observations, and the underlying chemical mechanisms remain only partially resolved.
Then, *what chemical events occur during charge formation and dissipation*?
In this work, we systematically and comparatively analyze the triboelectric behavior of bulk polymers and organic molecular powders. We use different contact and charging modes (simple contact and tapping) to measure the charge under different environmental conditions (temperature and humidity). We analyze the materials for physical, chemical, and mechanical changes that may have occurred before and after charging to detect surface chemical changes. The results indicate that charge generation in polymers is primarily governed by bond scission and material transfer at contacting interfaces. In contrast, the electrification of organic powders is influenced by a broader set of parameters, including crystallinity, crystal structure, particle size, and intrinsic molecular properties such as ionization energy and electron affinity. Finally, the chemical structure and reactivity underlie the contact charging of all organic materials. We believe that energy losses can be mitigated and more sustainable processes can be achieved by addressing triboelectrification problems with greater chemical insight.

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EES - D1 - O14
Regulating the interfacial electrochemical behavior of zinc anodes for stable aqueous zinc ion batteries

Yu Zhang[1]
[1]Dept. of Chemistry, Stockholm University, SE

Aqueous zinc ion batteries (AZIBs) have attracted great attention in electrochemical energy storage owing to their high safety, abundant zinc resources, and low cost. However, issues such as dendrite growth, corrosion, and side reactions hinder the stability of zinc anode, thereby limiting the cycling performance of AZIBs. To enhance the stability of zinc anode, we focused on regulating the interfacial electrochemical behavior and adopted strategies including epitaxial growth of the (101) crystal plane[1], bioinspired SEI construction[2] (Figure 1), and *in situ* gelation of electrolyte[3]. These approaches effectively optimized the Zn deposition/stripping process[4], suppressed corrosion and side reactions, and significantly improved the cycling stability of zinc anodes, thus enabling long-life operation of AZIBs.

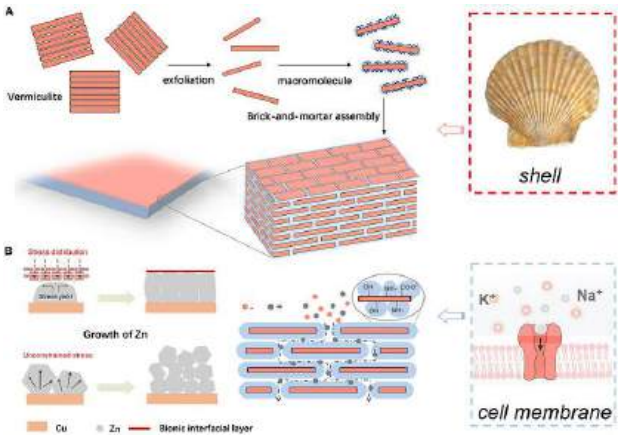

Fig. 1. Ultrastrong bioinspired "brick-and-mortar" artificial SEI for dendrite-free Zn anode[2]. (A) Schematic of preparation procedure; (B) ion transport channel structure and the inhibition effect to dendrite growth.

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EES - D1 - O15

Exploring Prussian blue as a safe-and-sustainable-by-design cathode material for sodium-ion batteries

Reja Trippaers[1,2,3], Dries De Sloovere[1,3], Karen Smeets[2], Marlies K. Van Bael[1,3], Nelly Saenen[2], An Hardy[1,3]
[1]Institute for Materials Research (IUMAT), Hasselt University, BE; [2]Centre for Environmental Sciences (CMK), Hasselt University, BE; [3]EnergyVille, BE

The growing demand for sustainable and safe energy storage solutions has accelerated research into sodium-ion batteries as an alternative to lithium-ion systems. Prussian blue analogues have emerged as promising cathode materials due to their low cost, environmental friendliness, biocompatibility, and favorable electrochemical properties. However, to ensure their safety, especially for vulnerable populations, it is essential to evaluate their potential toxicity alongside their electrochemical performance during the early stages of material design. Thirteen different Prussian blue particle samples were synthesized using a precipitation approach, systematically varying parameters such as flow rate, temperature, atmosphere, and the presence of ionic additives. The resulting materials were characterized using a comprehensive set of physicochemical techniques to determine particle size, crystal structure, water content, and Fe(II)/Fe(III) ratio, after which a subset was selected for parallel evaluation of electrochemical performance through rate capability testing and cellular effects, including cytotoxicity, proliferation, and differentiation capacity, in dental pulp stem cells. Our results show that maintaining a lower Fe(II)/Fe(III) ratio contributes to reduced cytotoxicity, and minimal effects on cell proliferation and differentiation capacity. Smaller particle size generally enhances electrochemical performance, although excessively small particles may increase toxicity. Additionally, higher crystallinity was associated with improved electrochemical behavior. Therefore, careful tuning of synthesis parameters to balance particle size and Fe(II)/Fe(III) ratio, alongside achieving good crystallinity, is crucial for developing Prussian blue cathode materials that combine high performance with minimal cytotoxicity. These design principles can guide the safe-and-sustainable-by-design development of Prussian blue-based cathodes for sodium-ion batteries.

EES - D1 - O16

Preparation and investigation of cross-linked polyacrylic acid-based hydrogel electrolytes in Zn–air batteries

Máté Benedek[1,2], Tamás Rácz[1], Dávid Nyul[1,2], Sándor Kéki[1], Tibor Nagy[1]
[1]Dept. of Applied Chemistry, University of Debrecen, HU; [2]Doctoral School of Chemistry, University of Debrecen, HU

In our research, we focused on the preparation and investigation of cross-linked polyacrylic acid-based hydrogel electrolytes for use in Zn–air batteries. The recipe described by Pei et al. [1] was used as a basis for the preparation of the polymer-based hydrogel electrolyte. We used *N,N'*-Methylene-bis(acrylamide) (MBAA) as crosslinker, adding it to acrylic acid in various concentrations (from 0.05 mol% to 0.75 mol%). After gelation, the crosslinked polyacrylic acid hydrogels were placed in solutions containing various concentrations of ZnO and KOH to swell. We performed electrochemical tests (PEIS, CED) on the swollen gels. The gel swollen in the solution with the lowest crosslink density and the lowest ZnO (0.05 M) and highest KOH (6 M) concentrations had the best electrochemical properties. The conductivity of this gel was 536 mS/cm. We also used the swollen gels in electrochemical full cells in Zn–air batteries. We designed and 3D-printed the cell housing from polypropylene, while we used active carbon containing poly(vinylidene fluoride) (PVDF) binder applied to Ni foam as the cathode. During the charge–discharge tests, we found that the cell assembled in this configuration operated for 32 hours, with a Coulomb efficiency approaching 100%, while the difference between the charge and discharge potentials was only 0.4 V. In addition, we performed experiments with a manganese-containing cathode according to the work of Liu et al. [2], during which we found that the cell assembled in this way operated as a battery for 55 hours, also with a Coulomb efficiency of nearly 100%. In addition, we determined the zinc transference number for swollen gels, which was found to be 0.90.

This work was supported by Project No. 2025-1.2.1-HU-RIZONT-2025-00006 has been implemented with the support provided from the National Research, Development and Innovation Fund of the Ministry of Culture and Innovation, financed under the 2025-1.2.1-HU-RIZONT funding program.

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EES - D1 - O17

Ambipolar donor-acceptor 2D covalent organic frameworks as cathode material for aluminum energy storage device

Cataldo Valentini[1*], Verónica Montes-García[1], Wojciech Kukułka[1], Saira Sarwar[1], Michał Bielejewski[2°], Mateusz Wlazło[3], Rossella Greco[4], Viktorija Pankratova[4], Ignacio Pérez Juste[5], Dawid Pakulski[1], Paolo Samorì[6], Artur Ciesielski[1,5]

[1]Centre for Advanced Technologies, Adam Mickiewicz University, PL; [2]Institute of Molecular Physics Polish Academy of Sciences, PL; [3]Chemical and Biological Systems Simulation Lab Centre of New Technologies University of Warsaw, PL; [4]Nano and Molecular Systems Research Unit, University of Oulu, FI; [5]Dept. of Physical Chemistry, Campus Universitario As Lagoas-Marcosende, Universidade de Vigo, ES; [6]Université de Strasbourg and CNRS, ISIS, FR

Lithium-ion batteries (LIBs) have become the dominant power source across various industries due to their superior energy density. However, the rising cost and limited availability of lithium resources pose significant challenges to the further development of LIBs, driving the search for alternative materials and more sustainable energy storage solutions.[1] Recently, aluminum-based ESS (Al-ESS) have garnered significant attention as a sustainable alternative for next-generation of ESS.[3] This interest stems from aluminum's high abundance, the use of non-flammable electrolytes, the high safety, low toxicity and outstanding theoretical volumetric capacity.[3–5] Therefore, the development of cathodes material that are able to host the sterically hindered aluminum ions (i.e. $AlCl_2^+$, $AlCl^{2+}$, $AlCl_4^-$, and Al_2Cl_7) is very coveted (Figure 1).[3,5,6] Among emerging materials, covalent organic frameworks (COFs) possess numerous advantages, such as presence of redox-active functional groups, defined pores structure, and high-surface area. However, the limited electrical conductivity of COFs makes essential the use of additives (such as carbon nanotubes) to increase the ions mass transport and electrical conductivity.

In this study, we focused on developing a 2D-COF formed by donor and acceptor building blocks with a strong charge transfer character, big pore size and high surface area, avoiding the use of carbon nanotubes. We employed as an electron donor tetrakis(4-aminophenyl)-1,4-phenylenediamine (TPA) and as an electron acceptor naphthalendiimide dialdehyde (NDI-DA) as the building blocks to synthesize functional COF TPA-NDI. The COF shows a Kagome topology with a high surface area (924 m^2/g) and well-defined pores with 1.6 nm and 3.4 nm size. Consequently, the COF TPA-NDI electrode achieves an unprecedent reported specific capacity of 270 mAh/g at a current density of 0.2 A/g, achieving a maximum energy density of 447 Wh/kg and a power density of 7 kW/kg. The Al-ESS shows more than 99% capacity retention after 5000 cycles at a current density of 5 A/g.

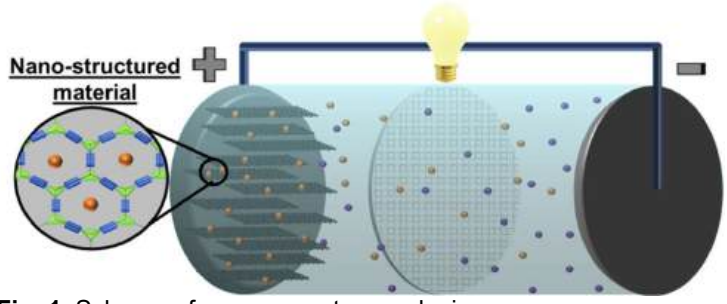

Fig. 1. Scheme of an energy storage device.

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EES - D1 - O18

Designing electrophoric covalent assemblies for molecular-level multielectron accumulation (charge pooling) and storage (in "reservoir" bonds)

Philippe P. Lainé[1], Éric Brémond[1], Magdaléna Hromadová[2]
[1]Université Paris Cité - CNRS, FR; [2]J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, CS

Fundamentally, electrical energy conversion and storage operate at the nanoscale, using electrons as elementary energy carriers and reactants. Beyond classical approaches for converting electrical energy into chemical energy for storage—such as in rechargeable batteries or electrocatalytic transformations for fuel production—it is noteworthy that (organic) Molecular Chemistry also holds promise for sustainably addressing the challenges in electrical energy storage.

At the molecular level, and from the standpoint of electrochemistry, it is worth distinguishing between multielectron accumulation (i.e., charge pooling), which is characterized by electrochemical reversibility, and multielectron storage (in chemical bonds), which is electrochemically irreversible but chemically reversible (hysteretic process).[1,2]

Depending on whether multielectron accumulation or storage is considered the functional target, molecular design is governed by different requirements. Both functions aim at managing intramolecular charge confinement, but they achieve this through different mechanisms, leading to distinct electrochemical behaviors and different potential technological applications. Molecular demonstrators of the “charge-pool” function (accumulation) can be regarded as prototypes of anolytes in RFBs, whereas demonstrators of the “charge-storage” function—relying on redox-switchable, scissile “reservoir bonds”—may serve as prototypes of electrode components for Organic Solid Batteries.

Here, we discuss design strategies developed to implement cooperative multielectron transfers—particularly “potential inversion”, which enables single-step two-electron transfer—in dedicated super-electrophoric covalent assemblies based on pyridinium-type redox-active components, which function as a “charge pool” (for charge accumulation) or an “electron reservoir” (for charge storage; see Figure below)[3–5].

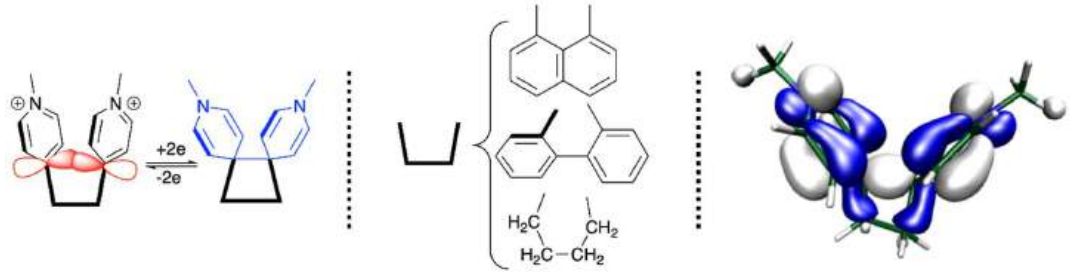

Fig. 1. Designing "reservoir bonds" (Structronic paradigm) for electron storage

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EES - D1 - O19

Greener peptide and PNA synthesis for high-value pharmaceuticals: from sustainable methodologies to industrially relevant APIs

Lucia Ferrazzano[1], Alessandra Tolomelli[1], Walter Cabri[1]
[1]Dept. of Chemistry "Giacomo Ciamician", Alma Mater Studiorum – University of Bologna, Italy

The transition of the pharmaceutical industry toward sustainable manufacturing requires synthetic methodologies that combine environmental responsibility with robustness, scalability, and regulatory compliance. This need is particularly urgent for peptide-based therapeutics, where the growing demand for highly potent and structurally complex APIs coincides with increasing pressure to reduce solvent toxicity, waste generation, and process mass intensity.[1]

Over the past five years, our research has integrated green chemistry principles into solid-phase, liquid-phase, and chemoenzymatic peptide synthesis, with a strong focus on industrial applicability. We developed eco-compatible solvent systems, alternative bases for Fmoc deprotection, and optimized coupling reagents that maintain high synthetic efficiency while improving sustainability and scalability.[2]

A key achievement is the selective elimination of side-chain protecting groups from arginine and histidine, enabling peptide assembly with improved atom economy and reduced impurity profiles. Using Oxyma Pure with tert-butyl ethyl carbodiimide for SPPS[3] and with N-(3-dimethylaminopropyl)-N′-tert-butylcarbodiimide for LPPS in green solvent systems, we established robust protocols for the synthesis of key intermediates of etelcalcetide and vasopressin, as well as fragments of high-value therapeutics such as liraglutide and tirzepatide. These methods are compatible with sequences containing unprotected arginine, histidine, tryptophan, and tyrosine residues.

Beyond peptides, these strategies were successfully extended to peptide nucleic acids, demonstrating a transferable framework for the sustainable manufacturing of high-value therapeutic molecules.

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EES - D1 – O20
Applying the SSbD concept in the development of biobased biodegradable polymers

Stefan Hahn[1], Franziska Breuer[1], Karsten Schlich[2], Camilla Braguglia[3], Maria Laura Di Lorenzo[4]
[1]Fraunhofer ITEM, Germany; [2]Fraunhofer IME, Germany; [3]CNR-IRSA, Italy; [4]CNR-IPCB, Italy

For the transition to more sustainable products, fossil-based polymers and harmful additives may be substituted with more biodegradable and less harmful alternatives. However, biodegradable and biobased polymers usually do not withstand high temperatures. The EU project BORN aims to develop a novel, bio-based and biodegradable polymer that, for the first time, can withstand temperatures of >100°C. In addition, the BORN material is intended to be circular, bio-based, biodegradable, compostable, food-safe, recyclable, and cost-effective – a combination that does not yet exist on the market. To achieve these objectives, BORN follows a holistic approach, from the development of sustainable material to the production of lab-scale prototypes and practical testing as food packaging. The revised framework on “Safe and Sustainable by Design (SSbD) Chemicals and Materials” will be used to evaluate and prioritize nature inspired polymers and additives. A novel, patentable crystal nucleating agent enables controlled crystallization during industrial processing and gives the polymer its exceptional temperature stability.
This talk will present the experience of applying the SSbD concept in BORN material development, which includes integration of new approach methodologies (NAM) to fill data gaps. In addition, the concept will be presented to evaluate its biodegradability in various real and extreme environments, complemented by ecotoxicity testing after biodegradation. For the comprehensive safety assessment, typical conditions on use and end-of-life must be defined, and emission or exposure estimated. BORN material allows a portfolio of applications which may include compostable microwavable containers for ready-to-eat meals, as well as low-cost cups for hot beverages. The material may be used also in agriculture (e.g. filler for mulching films), for reusable consumer goods, and for all applications where resistance to high temperatures is mandatory.

The EU project BORN (www.born-project.eu) is funded by Horizon Europe under the Grant Agreement number 101223095, Call HORIZON-EIC-2024-PATHFINDERCHALLENGES-01; doi: 10.3030/101223095

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EES - D1 – O21

Integrated biorefinery design and sustainability assessment for Butyric Acid production and separation from municipal solid waste

Keikhosro Karimi[1*], Ramon Ganigué[2], Joeri F.M. Denayer[1]
[1]Vrije Universiteit Brussel, Belgium; [2]Ghent University, Belgium; [2] Ghent University, Belgium

The valorization of municipal solid waste (MSW) into higher-value chemicals is critical for a circular bioeconomy[1]. This study presents a detailed process design and cradle-to-gate life cycle assessment (LCA) for producing butyric acid (BA) from MSW via an integrated biorefinery. The process comprises hydrothermal pretreatment[2], sequential lactic acid (LA) fermentation using *Lactobacillus rhamnosus*[3], butyric acid fermentation via a psychrophilic mixed culture[4], and product separation[5] (Figure 1). Due to the low concentration of BA, the separation constitutes a critical bottleneck, characterized by high energy demand and significant operational expense. Thus, two separation scenarios are rigorously compared: a novel adsorptive process using zeolite[6] (Scenario 1) and a conventional heat-integrated extractive distillation (Scenario 2, state-of-the-art benchmark)[5]. A comprehensive process model was developed based on laboratory data and scaled to handle the MSW at a commercial capacity.

The LCA results, following the ISO 14040/44 framework[7], indicate that the integrated biorefinery successfully converts waste into a valuable platform chemical with significant environmental impact benefits (Figure 2). A comparative analysis reveals a decisive environmental advantage for the novel adsorptive process. Scenario 1 reduces the long-term climate change impact (based on the Global Temperature Potential over 100 years, GTP100) by 35.5% compared to the conventional extractive distillation in Scenario 2. This substantial reduction in GHG emissions is directly linked to a 65-70% decrease in the thermal energy demand of the separation. The benefits of adsorptive separation extend across multiple impact categories: freshwater eutrophication is reduced by 37%, while damages to human health and ecosystem quality are lowered by 27% and 25%, respectively. The difference in water scarcity impact between the two scenarios is minor (<5%). This work demonstrates that coupling sequential fermentation with advanced, low-temperature separations like adsorption can significantly enhance the sustainability of waste-to-chemical pathways, providing crucial early-stage guidance for the design of environmentally superior circular biorefineries.

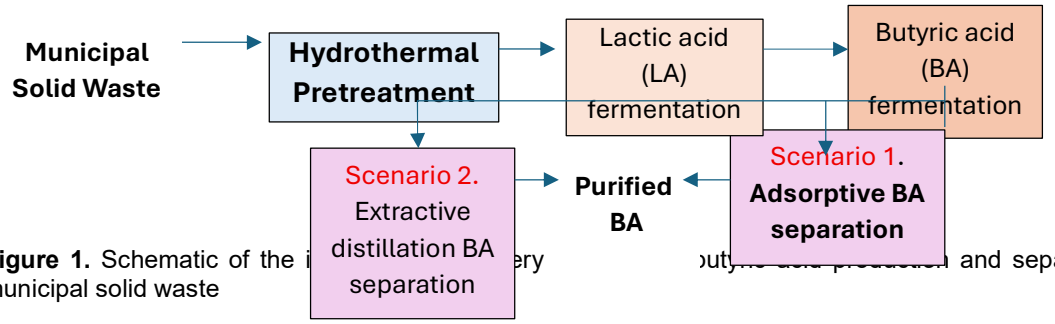

Figure 1. Schematic of the i ery utyric acid production and separation from municipal solid waste

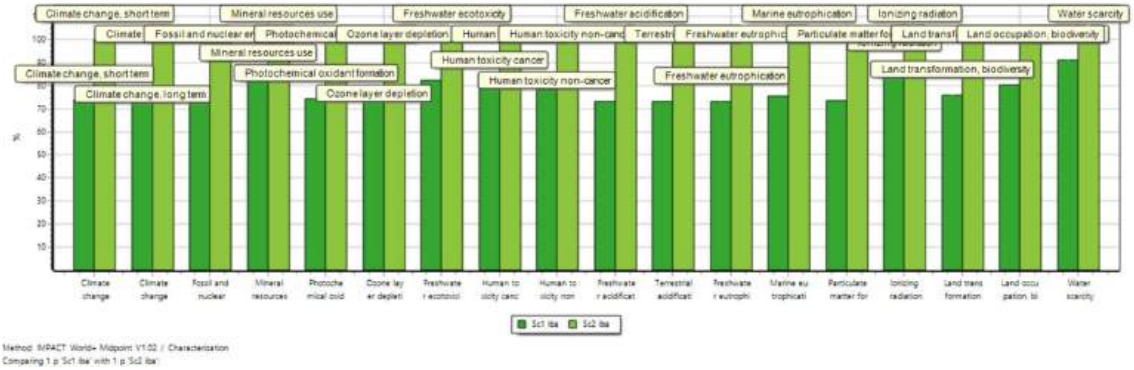

Figure 2. Midpoint impact assessment of Scenario 1 (adsorptive separation) and Scenario 2 (extractive distillation)

Acknowledgements: This work was supported by the Research Foundation - Flanders (FWO) through the Thematic Research Project *Effective.*

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EES - D1 – O22

Toward more sustainable silver-based antimicrobial materials: Life cycle assessment (LCA) of Silver-Nanoparticle Composites

Andrei Ungureanu[1,2], Antonella Sola[1,2,3], Davide Cattelani[1,3], Anna Maria Ferrari[1,2,3], Roberto Rosa[1,2,3]
[1]Dept. of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, Italy; [2]InterDept.al Center En&Tech, University of Modena and Reggio Emilia, Tecnopolo di Reggio Emilia, Italy; [3]InterDept.al Center for Applied Research and Services in the Advanced Mechanics and Motor Engineering Sector, InterMech–MO.R.E, Italy

The escalating global threat of antimicrobial resistance necessitates the continuous development of new antimicrobial strategies. Silver nanoparticles (AgNPs) have gained attention due to high surface-area-to-volume ratio, broad-spectrum activity, and ability to disrupt microbial membranes, generate reactive oxygen species, and induce DNA damage[1]. However, concerns regarding cytotoxicity and ecological risks limit their large-scale applicability.

Ag-based nanocomposites offer a promising alternative by enhancing antimicrobial performance while reducing silver content through synergistic interactions with metal oxides, carbon-based materials, biopolymers, or organic ligands. Despite their growing relevance, environmental evaluations remain scarce: only one Life Cycle Assessment (LCA) exists for pristine AgNPs[2], and none for Ag-based nanocomposites. LCA is an important tool for assessing environmental impacts across a product's life cycle—from raw material sourcing to end-of-life—supporting the design of more sustainable antimicrobial technologies.

This study applies LCA to compare the production of citrate-stabilized pristine AgNPs with several Ag-based nanocomposites, including MOF-based Ag/Copper(II) meso-tetra(4-carboxyphenyl)porphine (Ag/CuTCPP), Ag/anatase (Ag/TiO_2), Ag/nanocellulose, Ag/graphene oxide, Ag/$Ti_3C_2T_x$-MXene, and curcumin-based AgNPs (Cur-AgNPs). Impacts are compared not only per mass but also normalized to minimum inhibitory concentration (MIC), enabling a functional comparison of antimicrobial efficacy. Furthermore, the results are benchmarked against common antibacterial agents such as (–)-chloramphenicol.

The analysis underscores the importance of designing effective antimicrobials with low silver content. Cur-AgNPs (0.1% Ag) exhibit the lowest impacts across most categories, while Ag/$Ti_3C_2T_x$-MXene (74.5% Ag) shows substantially higher burdens. Despite containing only 1.4% Ag, Ag/CuTCPP presents elevated impacts in some categories due to the intensive solvent requirements for production. These findings highlight the need to concurrently optimize both composition and synthetic strategies for the development of novel antimicrobial silver-based nanomaterials.

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EES - D1 – O23

Rapid synthesis of nickel iron layered double hydroxide nanosheets for efficient oxygen evolution

Laura Fuentes-Rodriguez[1] , Judith Granados[1], Jan Plutnar[2], Ghazaleh Abdolhosseini[3], José Ramón Galán-Mascaros[34], Zdenek Sofer[2], Yolanda Cesteros[1], Bahareh Khezri [134]

[1] Universitat Rovira i Virgili, Spain; [2] University of Chemistry and Technology of Prague, Czech Republic; [3] Institute of Chemical Research of Catalonia, Spain; [4] ICREA, , Spain

Nickel–iron layered double hydroxides (NiFe-LDHs) are widely recognized as benchmark earth-abundant electrocatalysts for the oxygen evolution reaction (OER). However, their catalytic activity and durability remain highly sensitive to synthesis-controlled parameters, including layer stacking, surface composition and interlayer chemistry. Establishing clear structure–property relationships using more efficient and environmentally conscious synthesis strategies is therefore essential for their rational optimization.

In this contribution, we present a systematic comparison of four NiFe-LDH synthesis routes with a targeted Ni:Fe ratio of 3, in which two key parameters are independently tuned: (i) the coprecipitation regime, comparing conventional magnetic stirring with ultrasonic agitation, and (ii) the aging treatment, contrasting conventional reflux with microwave-assisted reflux. Notably, the proposed approaches significantly shorten synthesis times and improve energy efficiency compared to commonly reported methods, while preserving precise control over material composition. This experimental design enables decoupling the effects of mixing and thermal history on the physicochemical properties of the resulting materials. X-ray diffraction and transmission electron microscopy (Figure 1) confirm the formation of hydrotalcite-like two-dimensional hexagonal platelets in all samples. Complementary characterization by N_2 physisorption, thermogravimetric analysis, ICP-OES and X-ray photoelectron spectroscopy reveals route-dependent differences in mesoporosity, hydration degree and surface Ni/Fe ratios.

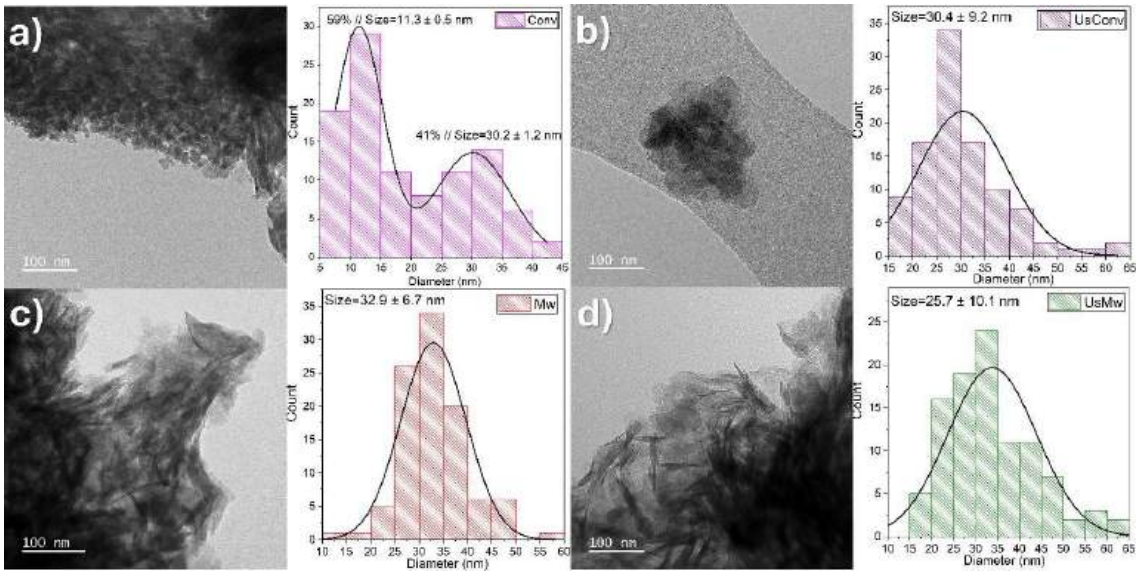

Figure 1. HRTEM images and particles size distribution of NiFe-LDH synthesized by a) conventional (100kX), b) ultrasound-conventional (100kX), c) microwave (120kX) and d) ultrasound microwave(100kX).

Electrochemical evaluation in 1 M KOH demonstrates that all NiFe-LDH catalysts significantly outperform bare Ni foam toward the OER (Figure 2). Overpotentials at 10 mA cm^{-2} (η_{10}) range from 259 to 297 mV, with the highest activity achieved for the ultrasound-assisted coprecipitation combined with microwave aging. In contrast, materials aged under conventional reflux display enhanced stability at higher current densities, reaching the lowest η_{100} value (319 mV). These results highlight an activity–durability trade-off linked to surface composition and metal leaching, while demonstrating that shorter, more sustainable synthesis routes can deliver highly competitive NiFe-LDH electrocatalysts.

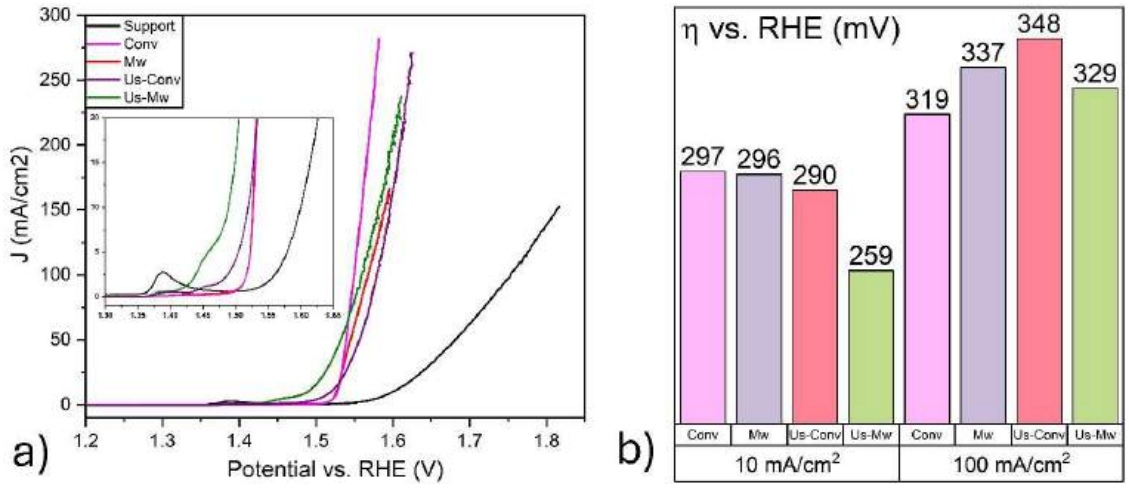

Figure 2. a) LSV curves, b) OER overpotentials of different samples at 10 mA cm^{-2} and 100 mA cm^{-2}

EES - D1 – O24

An in-depth study of the thermodynamics and kinetics of the structural phase transition of hydrothermally synthesized W/VO_2 microparticles

Stijn Cosemans[1,2], Elvan Heirman[1,2], Luc Leufkens[3,4], Marcel A. Verheijen[5,6], Ken Elen[1,2], Daniel Mann[1,3,4], An Hardy[1,2], Marlies K. Van Bael[1,2], Pascal Buskens[1,3,4]

[1]Institute for Materials Research (IMO), Hasselt University, Belgium; [2]imec vzw, IMOMEC Associated Laboratory, Belgium; [3]The Netherlands Organisation for Applied Scientific Research (TNO), The Netherlands; [4]Brightlands Materials Center, The Netherlands; [5]Dept. of Applied Physics, Eindhoven University of Technology, The Netherlands; [6]Eurofins Materials Science, The Netherlands.

Thermochromic VO_2 exhibits a reversible structural phase transition (SPT) from a semiconducting monoclinic VO_2(M) phase to a metallic rutile VO_2(R) phase near 68 °C, accompanied by a modulation in solar infrared (IR) transmittance.[1,2] This makes VO_2 a promising material for smart windows.[3] However, the high intrinsic transition temperature (T_0) and optical limitations of bulk VO_2 have driven extensive efforts to lower T_0 and improve phase transition behavior through metal doping and particle engineering.[4,5]

Here we investigate the thermodynamic and kinetic properties of the SPT of hydrothermally synthesized W/VO_2 microparticles to determine whether they are suited for smart window applications. A hydrothermal method was used to produce VO_2(M) with W concentrations between 0.5 and 2.5 at.%.[2] Differential scanning calorimetry (DSC) was employed to determineT_0, switching enthalpy (ΔH_{spt}), hysteresis width and hysteresis gradient, while isoconversional kinetic analysis was used to determine the activation energy E_A of the SPT.

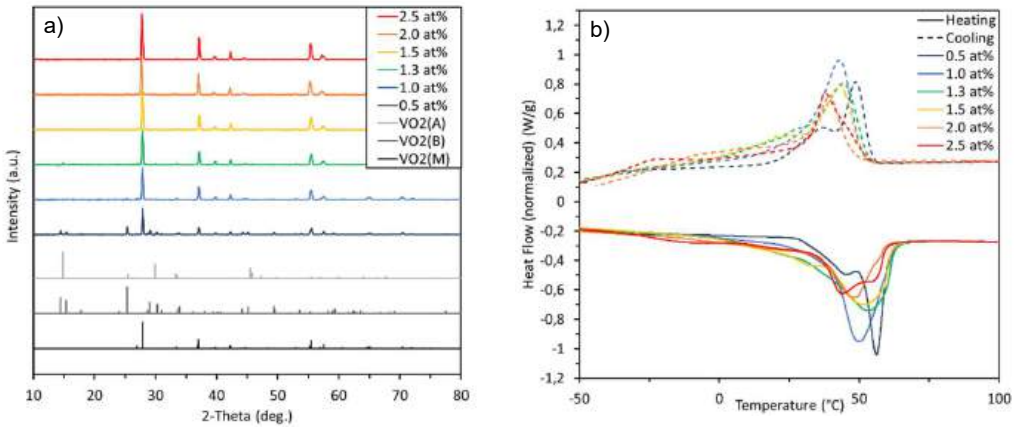

Fig. 1. (a) Powder X-ray diffractograms and (b) DSC analyses of W/VO_2 microparticles comprising 0.5 at.% to 2.5 at.% W.

XRD confirms formation of VO_2 (Fig. 1a), while DSC shows a decrease in T_0 with increasing tungsten content (Fig. 1b). Scanning electron microscopy revealed rod- and asterisk-shaped morphologies larger than 1 µm. DSC peaks were very broad, due to a broad particle size distribution and inhomogeneous W incorporation. The kinetics of the SPT were studied using Friedman's differential isoconversional method.[5] The results showed that E_A rapidly decreased with an increasing difference between the temperature of the powder and T_0 (Fig 2). E_A was of the same order of magnitude as reported for bead-milled W/VO_2 powders.[6]

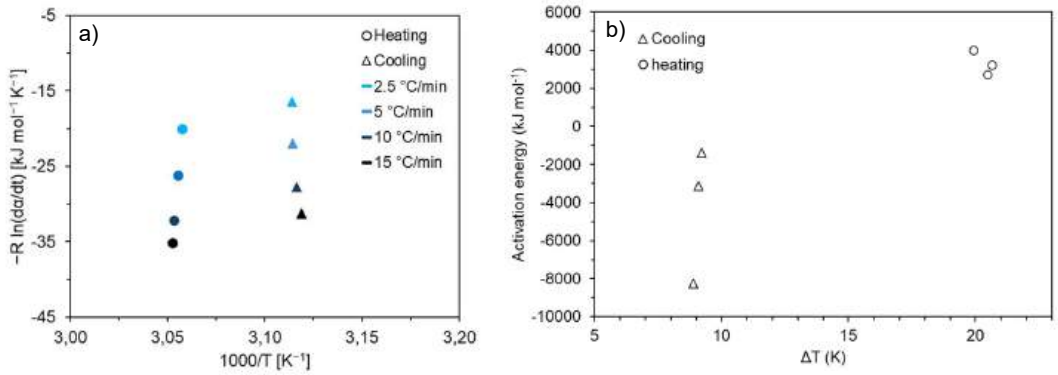

Fig. 2. (a) Friedmann plot for W/VO_2 microparticles (0.5 at-% W) at 50% conversion, (b) activation energy as a function of the difference between the temperature of the powder and T_0.

This temperature-dependence of the activation energy indicates that the formation of new nuclei in the original phase determines that rate of the SPT. The thermodynamic and kinetic characteristics of the SPT of hydrothermally synthesized W/VO_2 are similar to milled W/VO_2, and can be used in thermochromic smart windows.[6]

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EES - D1 - F01

Activated ester-functionalized poly(ethylene terephthalate) for degradable epoxy thermosets and recyclable carbon fiber composites

Dula Daksa Ejeta[1], Hou-Wei Lee[1], Hsin-Ting Liu[1], Wei-Yi Wu[1], Ching-Hsuan Lin[1]
[1]Dept. of Chemical Engineering, National Chung Hsing University, Taichung, TW

Poly(ethylene terephthalate) (PET), one of the most widely sourced recyclable plastics, presents both a sustainability challenge and an opportunity for innovative carbon reduction strategies. Building on our previous finding that epoxy groups can undergo insertion with carbonate or activated esters [1], we recognized that PET, as a non-activated ester, requires structural modification to enable such reactivity. In this study, we established a PET recycling strategy by introducing activated ester functionalities into its backbone (Figure 1). Commercial PET and polycarbonate (PC) were first employed to optimize transesterification and curing systems, which were later extended to waste PET and PC. Zinc acetate catalyzed transesterification enabled incorporation of activated ester moieties from PC into PET, yielding PET/PC copolymers (T5 and T3; PET/PC = 5:5 and 3:7 wt %). These copolymers were subsequently cured with BPA-epoxy resin (EP) under different catalysts. Among them, tetrabutylphosphonium bromide (TBPB) afforded the best performance, with T3/EP and T5/EP exhibiting glass transition temperatures of 161 °C and 152 °C, tensile strengths of 96 MPa and 78 MPa, and excellent thermal stability (Td5% > 400 °C, char yields up to 18%). Carbon fiber composites prepared from T3/EP and T5/EP were successfully depolymerized via aminolysis, yielding a cyclic tetraol that was reutilized for polyurethane synthesis. The recovered carbon fibers, characterized by SEM, EDS, Raman spectroscopy, and tensile testing, retained both surface quality and mechanical integrity. This work demonstrates that activated ester functionalization enables efficient recycling of PET into high-performance, degradable epoxy thermosets and recyclable carbon fiber composites. The approach not only mitigates plastic waste but also advances circularity in high-value materials.

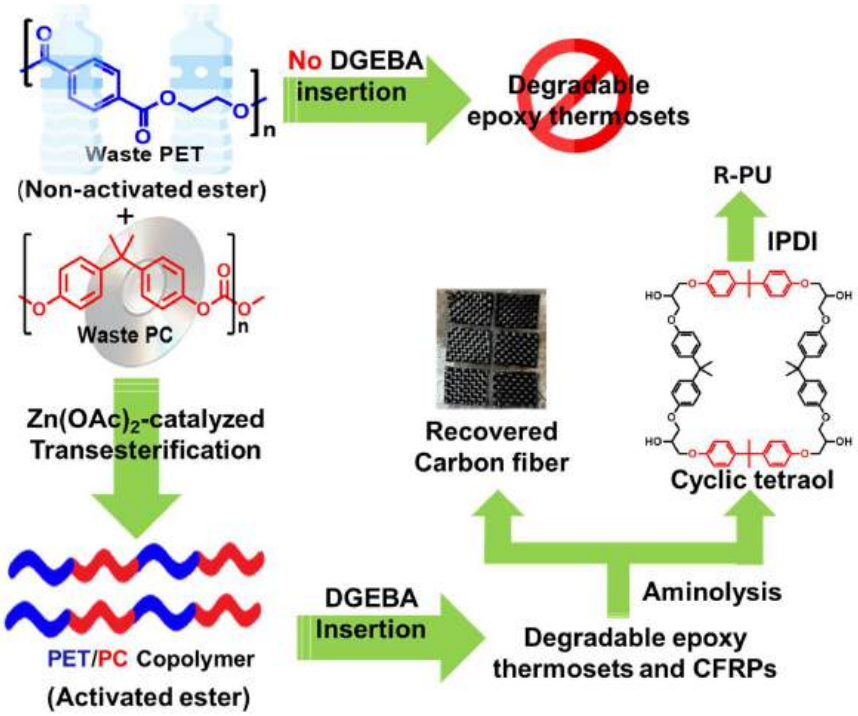

Fig. 1. Schematic illustration of the recycling strategy developed in this work.

Acknowledgements: This work was financially supported by the National Science and Technology Council (NSTC) (112-2221-E-005-005-MY3) and Featured Area Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (113L9006), Taiwan.

Reference:
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EES - D1 - F02

Photothermal/photocatalytic activation of peroxymonosulfate using $SrFe_{12}O_{19}$@Ni-P core@shell microparticles for energy efficient water remediation

Jordi Rigual-Miret[1,2], Queralt Bautista[1,2], Arnau Fons[3,4], Josep Nogués[3,5], Elvira Gómez[1,2], Borja Sepúlveda[4], Albert Serrà [1,2]

[1]Grup d'Electrodeposició de Capes Primes i Nanoestructures (Ge-CPN) – Universitat de Barcelona, ES; [2]Institute of Nanoscience and Nanotechnology (IN²UB) - Universitat de Barcelona, ES; [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Barcelona, ES; [4]Institut de Microelectrònica de Barcelona (IMB-CNM, CSIC), Campus UAB, Barcelona, ES; [5]ICREA, ES

Contamination of water resources with persistent organic compounds, including pharmaceuticals, has emerged as a major environmental concern due to their frequent presence, limited biodegradability, and potential risks to ecosystems and human health. The urgent need for more efficient water remediation systems requires the development of new, low cost and low energy strategies to remove those persistent organic pollutants. However, current technologies often involve high energy demand or lead to incomplete mineralization, which makes multi-step treatment processes necessary.

This study addresses a critical challenge in the field of advanced oxidation processes (AOPs) by developing an efficient catalytic process for the degradation of organic residues in water through the activation of peroxymonosulfate (PMS), using Ni-P-coated $SrFe_{12}O_{19}$ microparticles. The synthesized particles were subjected to thermal, photothermal and photocatalytic conditions by conventional heating or light (near-infrared or blue) actuation as well as concentrated solar illumination.

The results demonstrated that the activation using blue light outperformed conventional thermal treatments or photothermal near-infrared actuation, enhancing the PMS decomposition at moderate temperatures and leading to a 99.9% degradation and 99.7% mineralization of tetracycline in 90 min as well as achieving up to 76.2% mineralization of a 120 ppm multi-pollutant solution in 90 min, with markedly lower energy requirements than the conventional heating activation. In the different processes evaluated, catalysts maintained high activity over multiple cycles with negligible metal leaching.

These findings highlight the potential of $SrFe_{12}O_{19}$@Ni-P microparticles for efficient, reusable, and low-energy advanced oxidation processes, and solar-compatible wastewater treatment applications, presenting a scalable alternative to conventional heating strategies.

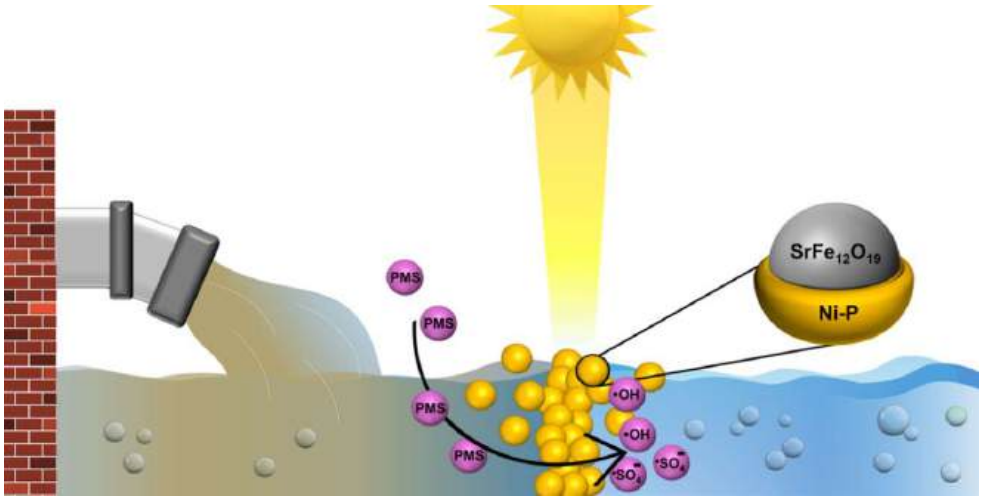

Fig. 1. Schematic representation of PMS activation and pollutant degradation over $SrFe_{12}O_{19}$@Ni-P under sunlight.

Acknowledgements: The authors would like to express their gratitude to the Departament de Recerca i Universitats, particularly the Departament d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR).

EES - D1 - F03
Acid−modified MXenes as catalysts for upcycling PET by hydrolysis

Maria-Iuliana Chirica[1,2], Anca Mirea[1], Andrei Kuncser[1], Stefan Neatu[1], Mihaela Florea[1], Michel W. Barsoum[3], Florentina Neatu[1*]
[1]National Institute of Materials Physics, RO; [2]University of Bucharest, Faculty of Physics, RO; [3]Dept. of Materials Science and Engineering, Drexel University, USA

The increasing gathering of polymeric waste has intensified environmental concerns, challenging the sustainability of plastics in modern society. Although heterogeneous catalysis represents a promising approach for plastic recycling, current catalytic systems still undergo from limited efficiency, preventing their large-scale industrial implementation[1,2]. In this study, a new class of solid acid catalysts is proposed for the catalytic depolymerization of polyethylene terephthalate (PET) into its constituent monomers. MXenes, an emerging family of two-dimensional transition metal carbides and nitrides with graphene-like architectures, offer a versatile platform due to their tunable surface chemistry and layered structure. These materials are obtained by selective etching of the A element from MAX phases[3,4].
Herein, the catalytic properties of MXenes were tailored through surface functionalization with sulfonic acid groups, achieved by grafting sulfanilic acid moieties onto $Ti_3C_2T_x$ sheets[5]. A series of sulfonated MXenes with varying acid loadings was synthesized, denoted as $Ti_3C_2T_x$–SO_3H–y (y=1,3,5,7), corresponding to the amount of sulfanilic acid used in the preparation of the catalyst. Structural and morphological analyses using XRD, DRIFT, Raman spectroscopy, SEM, and TEM confirmed the preservation of the lamellar MXene structure after sulfonation process, accompanied by an increase in interlayer spacing due to the insertion of aryl sulfonate groups. The successful incorporation of –SO_3H functionalities was further validated by EDX and XPS measurements.
The sulfonated MXenes exhibited excellent catalytic activity in PET depolymerization by hydrolysis, achieving up to 99% isolated yield of terephthalic acid (TPA) for the catalyst with the highest sulfonic acid content. The influence of reaction parameters, including temperature, pressure, and catalyst loading, highlights $Ti_3C_2T_x$–SO_3H–y as a highly efficient and environmentally friendly catalyst for PET upcycling.

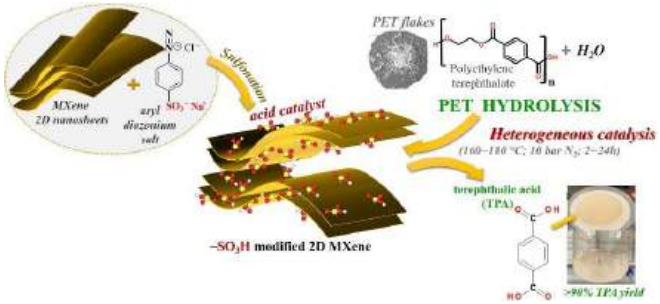

Fig. 2. Schematic representation of the catalytic PET depolymerization process using sulfonated MXenes as catalyst through hydrolysis reaction.

Acknowledgement: This work was supported by Romanian Ministry of Education and Research through the Core Program 2023–2026 (contract PC3–PN23080303); IMC, AGM and MF acknowledge the CNCS/CCDI-UEFISCDI for the COFUND-NEXT-PEMFC project, within PNCDI IV.

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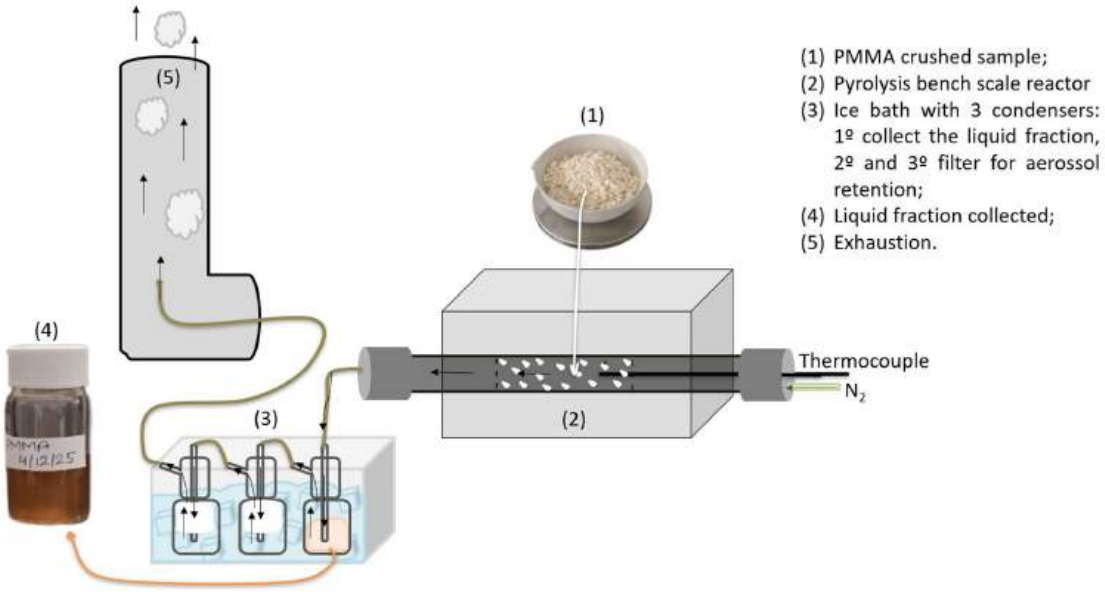
EES - D1 - F04

Valorization of poly(methyl methacrylate) waste through pyrolysis

Patrícia Mata[1], Shantanu Wahane[1], Inês Almeida[2], Sofia Caldas[2], Flávio Azedo[3], Jorge Marinheiro[3], Ana Barros-Timmons[2], Nuno Gama[2], Luís A.C. Tarelho[1]

[1]Dept. of Environment and Planning, Centre for Environmental and Marine Studies (CESAM), University of Aveiro, PT; [2]Dept. of Chemistry, Institute of Materials (CICECO), University of Aveiro, PT; [3]Porcelanas da Costa Verde S.A., PT

Poly(methyl methacrylate) (PMMA) is thermoplastic widely used in several industrial applications. Its high thermal stability, presents a significant end-of-life management challenge. Mechanical recycling is limited, particularly for mixed or contaminated waste streams, and chemical routes remain scarcely implemented at industrial scale. Consequently, a substantial fraction PMMA of still ends in landfill or incineration. The CiPoCer project investigates chemical recycling approaches to recover high-value resources and reintegrate them into a circular materials strategy. Among other technologies, pyrolysis stands out for its potential to convert PMMA waste into chemical products that can be integrated in materials recycling loops. The thermal behavior of PMMA is particularly favorable to the formation of liquid fractions under controlled conditions, creating an opportunity for methyl methacrylate (MMA) recovery[1]. In this context, preliminary bench-scale experiments were carried out in a temperature range of 500ºC to 600°C, solid residence times of 5 to 30 minutes, and heating rates of 10 to 30°C/min. The objective at this stage is to understand the basic thermochemical behavior of the specific PMMA under pyrolysis conditions and establish appropriate experimental boundaries to support a more detailed study. In this work are presented preliminary experimental results, namely, the yield of liquid (oil) fraction. It was observed that at 550°C and 30ºC/min, the solid-to-liquid conversion reached approximately 90%, with negligible char or wax formation. In contrast, at 500°C and 10°C/min, the yield dropped to <50%, with substantial wax formation. These results constitute the first mapping of PMMA pyrolysis behavior within the CiPoCer project and provide the experimental basis for defining a deeper study of the process.



Acknowledgements: This work was supported by the FEDER – European Regional Development Fund, through the Innovation and Digital Transition program of the "CiPoCer" project, COMPETE2030-FEDER-01195100. P. Mata received a research fellowship from the "CiPoCer" project (BI/UI89/12618/2025).
This work was developed within the scope of the project CICECO Aveiro Institute of Materials, UID/50011/2025 (DOI 10.54499/UID/50011/2025) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).
This work was funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project CESAM-Centro de Estudos do Ambiente e do Mar, references UID/50017/2025 (doi.org/10.54499/UID/50017/2025) and LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020).

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EES - D1 - F05

Pollen-based photothermal catalysts: A sustainable platform for advanced removal of organic pollutants and microplastics

Pol Vilariño[1,2], Queralt Baustista[1,2], Elvira Gómez[1,2], Albert Serrà[1,2]
[1]Grup d'Electrodeposició de Capes Primes i Nanoestructures (GE-CPN), Dept. de Ciència de Materials i Química Física, Universitat de Barcelona, ES; [2]Institute of Nanoscience and Nanotechnology (IN[2]UB), Universitat de Barcelona, ES

The removal of persistent organic pollutants and microplastics from water remains a major challenge, calling for efficient and sustainable catalytic materials. This work presents the first application of pollen-based biohybrid catalysts (previously developed for photothermal biomass valorization) for advanced water decontamination under UV/visible light irradiation and peroxymonosulfate (PMS) activation. Nine catalysts were prepared by electroless deposition of Ni, Ru, or Cu onto three natural pollen substrates (*Salix caprea (SC)*, *Sambucus nigra (SN)*, *Helianthus annuus (HA)*), whose intrinsic hierarchical porosity, high surface area, and strong light absorption significantly enhance catalytic performance.

Among all materials, Cu-coated *Helianthus annuus* pollen (Cu/HA) exhibited the highest activity toward sulfamethoxazole (SMX, 20 ppm) degradation, achieving 98–100% pollutant removal within 60 min and 60–75% total organic carbon (TOC) reduction after 180 min. In multicomponent systems containing SMX, ibuprofen, levofloxacin, and tetracycline, Cu/HA maintained >90% overall pollutant removal, with only marginal losses when operating in tap water, demonstrating remarkable robustness against real-water matrix effects.

The catalysts also showed promising activity toward microplastic degradation. Polystyrene particles (100 nm–10 µm) exhibited 20–40% size reduction and clear surface erosion after UV/PMS treatment, as evidenced by SEM, TEM, and DLS analyses – consistent with efficient sulfate radical generation and the strong photothermal response of the pollen scaffolds.

Overall, these results position metal-functionalized pollen as a low-cost, recyclable, and high-performance alternative to conventional photocatalysts. Their combined photothermal and radical-driven reactivity, broad UV responsiveness, and compatibility with PMS highlight their potential for scalable water purification technologies aligned with circular-economy principles.

Keywords: water decontamination, biohybrid catalysts, electroless deposition, microplastic degradation.

Acknowledgements: Grant CNS2024-154690 funded by MICIU/AEI/10.13039/501100011033 and, as appropriate, by "ESF Investing in your future", by "ESF+" or by "European Union NextGenerationEU/PRTR". The authors also would like to express their gratitude to the Departament de Recerca i Universitats, particularly the Departament d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR) for their support. Authors thank the CCiT-UB for the use of their equipment.

EES - D2 - O01
Electrified carbon capture by adsorption: Linking Adsorbent formulation, structure, and regeneration behavior

Mohsen Gholami[1], Tom R.C. Van Assche[1], Joeri F.M. Denayer[1]
[1]*Vrije Universiteit Brussel, BE*

The decarbonisation of industrial separations requires not only new adsorbent materials, but also novel regeneration strategies compatible with low carbon and intermittent energy supply. In adsorption based carbon capture, electrification of the regeneration step provides a direct pathway to reduce fossil derived heat demand while enabling rapid and controllable energy input[1]. This presentation addresses electrified carbon capture from a materials development perspective, highlighting how adsorbent formulation and shaping govern both adsorption performance and electrified thermal response.
Electrically responsive adsorbents are developed through composite formulation, structuring, and shaping approaches that preserve the intrinsic CO_2 selectivity of established materials, such as zeolites and functionalized porous solids, while enabling efficient Joule and induction heating [2,3]. Shaping into monolithic architectures creates continuous conductive networks and modifies heat and mass transport at the mesoscale, allowing deliberate tuning of electrical resistivity, thermal response, and mechanical integrity [1]. Comprehensive characterization is performed combining adsorption equilibrium and kinetic measurements with textural, structural, and electrical analyses (Figure 1). In situ monitoring of temperature and electrical behavior during regeneration provides insight into the coupling between adsorbate loading, heat generation, and desorption kinetics under electrified conditions (Figure 2).
The results demonstrate that adsorbent shaping and composite design, often regarded as downstream adsorbent processing steps, become key chemical design variables in electrified carbon capture. This work links molecular properties to macroscopic electrified thermal swing adsorption process, demonstrating how materials properties can directly enable more energy-efficient and sustainable carbon capture technologies.

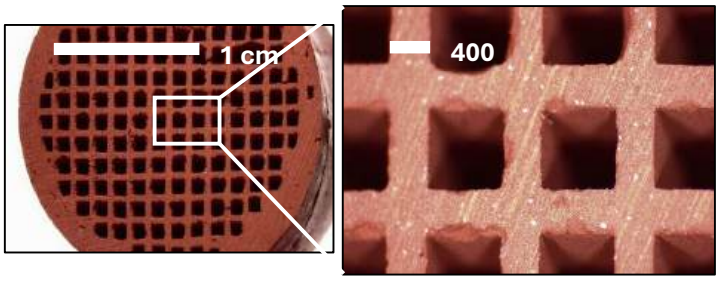

Fig. 1. Images of conductive monolith heated by Joule heating.

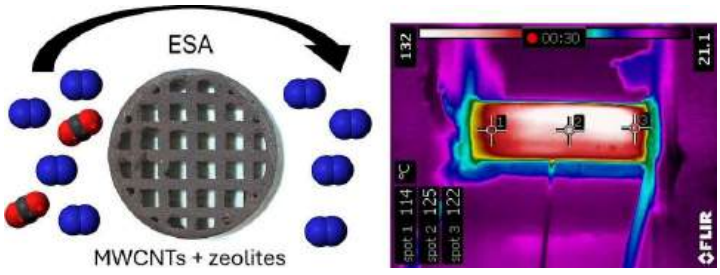

Fig. 2. Images of induction susceptible monolith

The authors would like to acknowledge VLAIO for the financial support (HBC.2021.0255).

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EES - D2 - O02
Hierarchical porous silicas with tunable porosity for CO_2 capture and separation

G. Rodríguez-Almaguer[1], R. Backov[2], V. Fierro[3], P. Bordat[1], D. Broseta[1]
[1]Laboratoire des Fluides Complexes et leurs Réservoirs, CNRS, UPPA, FR; [2]Centre de Recherche Paul Pascal (CRPP), CNRS, Université de Bordeaux, FR; [3]Institut Jean Lamour, CNRS, Université de Lorraine, FR

Industrial flue gases and raw biogas require sorbents that combine high CO_2 uptake, strong selectivity, fast kinetics, and low-grade heat regeneration[1]. We present a family of silicas at multiscale porosity synthesized via a simple sol–gel route, coupled with supercritical CO_2 drying (aerogels), ambient evaporation (xerogels), or high-internal-phase emulsion (HIPE) templating (macrocellular foams)[2]. By tuning precursor pH and Zr/Al doping, we adjust the fractions of macro-, meso-, and micro-/ultra-micropores. N_2 sorption yields SSA > 1000 $m^2\ g^{-1}$; SAXS confirms a mass-fractal network; TGA shows < 12 % mass loss up to 600 °C, indicating thermal stability. At 50 °C and 1 bar, Si–Zr xerogels adsorb ~33 kg $CO_2\ m^{-3}$, while ultralight foams adsorb ~2 kg $CO_2\ m^{-3}$. The volumetric capacity of xerogel SiZr-7 reaches ~150 kg m^{-3} at 10 bar/298 K, exceeding those of other porous silicas under identical or comparable conditions. Correlations show low-P&T capture is driven by ultramicroporosity, shifting to A_{BET}/micro–mesopore control at higher P (Fig. 1). For micro/mesoporous xerogels, ideal selectivity reaches up to 75–50 (post-combustion, 15 vol % CO_2/N_2, 1 bar, 25–50 °C) and 14.5–9.8 (biogas, 40 vol % CO_2/CH_4, 1–10 bar, 25 °C); isosteric heats < 35 kJ mol^{-1} ensure low-energy regeneration. Conversely, pre-loaded humidity (≤ 20 % RH) reduces the CO_2 capacity at 323 K by ≤ 80 % across all silicas (gravimetric CO_2/H_2O co-adsorption). These preliminary results warrant further study toward next-generation CCS materials.

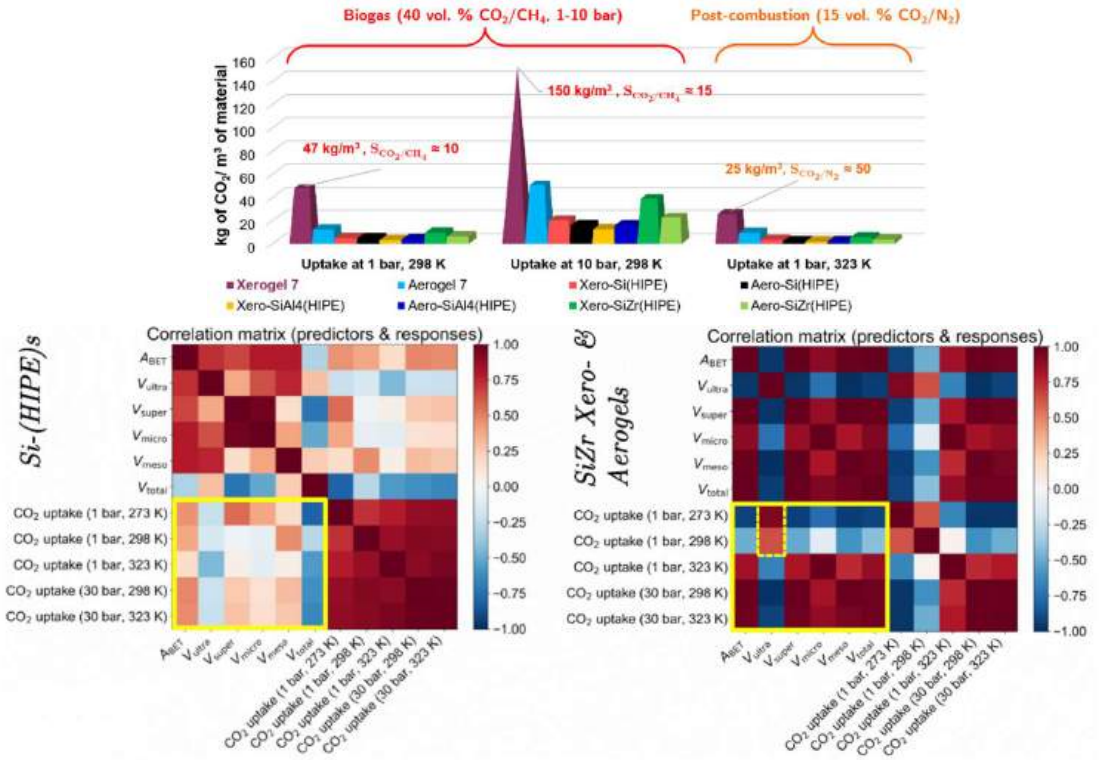

Fig. 1. Volumetric CO_2 uptakes and ideal selectivity at different CCS scenarios; low-P equilibrium driven by <0.7 nm pores; high-P by surface and micro–meso volume.

Acknowledgements: This work was supported by the **CATALPA project** (PEPR **SPLEEN**, France 2030 "Decarbonation of industry"), by **COSMICC** (Carnot **ISIFoR**), and by the **EDENE Doctoral Program** (Marie Skłodowska-Curie **COFUND**, Horizon 2020) at Université de Pau et des Pays de l'Adour (UPPA).

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EES - D2 - O03

Zr-doped $Ti_3C_2T_x$ MXene for enhanced CO_2 capture and efficient catalytic conversion to value-added products

Deeksha Jaiswal[1], Jitendra Kumar Bera[2], Jayant Kumar Singh[1]
[1]Dept. of Chemical Engineering, Indian Institute of Technology, IN; [2]Dept. of Chemistry, Indian Institute of Technology, IN

The global effort towards achieving net-zero emissions motivated researchers to develop advanced strategies for the reduction of carbon dioxide (CO_2) emissions from industrial sectors, with a key focus on capturing CO_2 from flue gas and converting it into valuable products. In this context, we have synthesized a novel Zr (Zirconium) doped titanium-based MXene via etching Al (Aluminum) layers from the MAX phase, followed by hydrothermal doping of Zr on MXene layers (see Figure 1) for CO_2 adsorption and catalytic conversion. The incorporation of Zr into the MXene layers creates additional active sites and improves binding interactions with CO_2 molecules, leading to increased surface area and CO_2 adsorption capacity. Beyond adsorption, the Zr@MXene material exhibits exceptional performance in the catalytic conversion of CO_2 with epoxides to cyclic carbonates, achieving nearly 99% yield for styrene carbonate, an industrially relevant solvent, along with high yields for other substituted epoxides. Density functional theory (DFT) was performed to gain a better understanding of the reaction mechanism. The result indicates a feasible cyclo-addition pathway with an energy barrier of 35.7 kcal/mol (Figure 2). The reaction was exothermic in nature, supporting potential for energy-efficient CO_2 utilization.

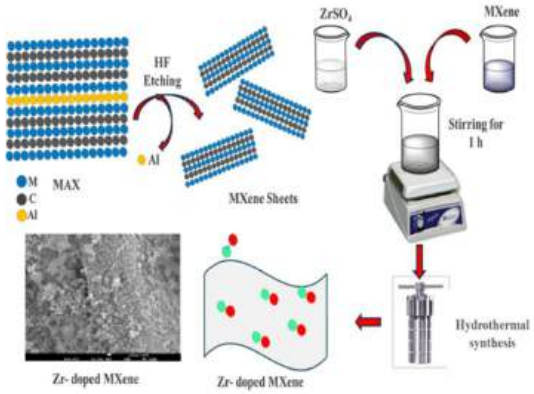

Fig. 1. Schematic illustration of the synthesis procedure of Zr@MXene

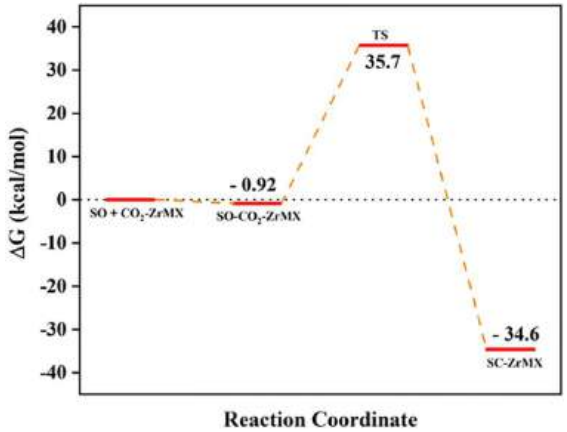

Fig. 2. Energy profile diagram for the cycloaddition reaction pathway

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EES - D2 - O04

Resol resin-derived carbon embedded in mesoporous magnesia nanocrystalline sorbents for highly efficient CO_2 capture and multiple regeneration performances

Adel A. Ismail[1*], L. A. Al-Hajji[1], Saad Makhseed[2], Ahmed Abdel Nazeer[1], A. Joseph[1], M. Alsaidi[1], S. A. Ahmed[1]
[1]Nanotechnology Applications Program, Energy & Building Research Center, Kuwait Institute for Scientific Research (KISR), K; [2]Dept. of Chemistry, Kuwait University, KW

As emissions rise, so does interest in developing new ways and materials that absorb CO_2 before or after it is released into the environment. Adsorption is unique among CO_2 capture systems because it provides high-purity streams that are easy to utilize and need little energy. As a result, many adsorbent materials have been developed expressly for this application. In this study, various carbon-embedded magnesium oxide porous materials (C@MgO nanocomposites) were synthesized using F127 surfactant and Resol Resin as a carbon source via a sol-gel process, enabling high-efficiency CO_2 capture. The homogeneous multicomponent mixture is transferred to dishes and placed in an oven at 30–40 °C for 24 h to remove ethanol by evaporation. The as-made products were calcinated in a tubular furnace at 500 °C, 600 °C, 700 °C, and 800 °C for 2h under N_2 to obtain mesoporous C@MgO nanocomposites. The obtained C@MgO nanocomposites were investigated by XRD, XPS, FT-IR, N_2 isotherms, and TEM. The findings showed that adding resol and surfactant improved the crystallinity of the produced MgO NPs. Interestingly, the C@MgO-600 displayed remarkable crystallinity with no impurities. Because of its greater porosity and reactive surface sites, the obtained C@MgO's distinctive textural features can improve adsorption capacity. The results showed that C@MgO-600 had the maximum CO_2 adsorption capacity of 4.12 mmol/g, which exhibits a larger adsorption capability, 10.8 times that of pure MgO (0.38 mmol/g). The addition of surfactant and Resol produces porous nanostructured MgO with numerous defects, small crystallite size, and a large surface area, thereby significantly increasing CO_2 adsorption capacity compared with bulk MgO. Additionally, after five adsorption/desorption cycles, C@MgO-600 retained 82.5% of its adsorption capacity, demonstrating its enormous potential for efficient CO_2 capture application and providing a viable way to lower CO_2 emissions.

Acknowledgements: The financial support received by the Kuwait Foundation for the Advancement of Sciences (KFAS) under contract number: PR23-42SC-1839. Kuwait Institute for Scientific Research (KISR) is gratefully acknowledged for the instrumental facilities.

EES - D1 - O05

Porphyrin molecular mediators enhancing the hydrogenation of CO_2 at the liquid-solid interface for Cu_xAu_y/ZnO catalysts

Hung Mac[1], Soufiane Bahou[1], Noora Piash[1], Katja Neubauer[1], Ali M. Abdel-Mageed[1]
[1]Leibniz Institute for Catalysis (LIKAT), DE

Background: Building chemicals from CO_2 is essential to reduce carbon-footprint and to establish sustainable economy.[1] Liquid-phase CO_2 hydrogenation on heterogeneous catalysts s particularly attractive process for green CO_2 reduction under thermal or photo-thermal conditions, yet limited by low gas solubility and interfacial reactants transport .[2] Adopting strategies to enhance gas transfer to the liquid–solid interface is therefore critical for scaling this process. In our recent work, bimetallic Cu_xAu_y/ZnO catalysts showed excellent activity and methanol selectivity for CO_2 reduction in liquid water.[3] Expanding these finding, we employed porphyrin-derived complexes (chlorophyllin) to enhance CO_2 transfer to the Cu_xAu_y/ZnO interface and improve its hydrogenation to methanol.
Experimental: Catalytic measurements were carried out in a 45 mL autoclaves[CO_2:H_2 = 1:3 (50 bar/ 160 °C, pressurized in 5 ml water and using optimized $Cu_{93}Au_7$/ZnO catalyst[3, 4]). EPR spectroscopy and zeta potential measurements were used to elucidate the origin of catalytic activity and related surface charge dynamics.
Results: Addition to an optimum concentration of chlorophyllin (0.01 $g_{chlorophyllin}$ L^{-1}) in water was demonstrated to maximize CO_2 solubility in water. Catalytic activity in the absence and in the presence of chlorophyllin in water showed only methanol as a single product, without any side gas products (**Fig. 1a).** CO_2 conversion in the presence of the molecular mediator increased by a factor between 2 and 3 depending on total metal loading. Spin-trap EPR studies (**Fig. 1b**) show that chlorophyllin enhances CO_2 solubility, strengthens electrostatic interactions with the surface, and promotes the formation of C-centered and OH radicals during CO_2 hydrogenation. These results support the development of hybrid systems integrating CO_2 capture and valorization and improve understanding of CO_2 interactions at liquid-solid interfaces.

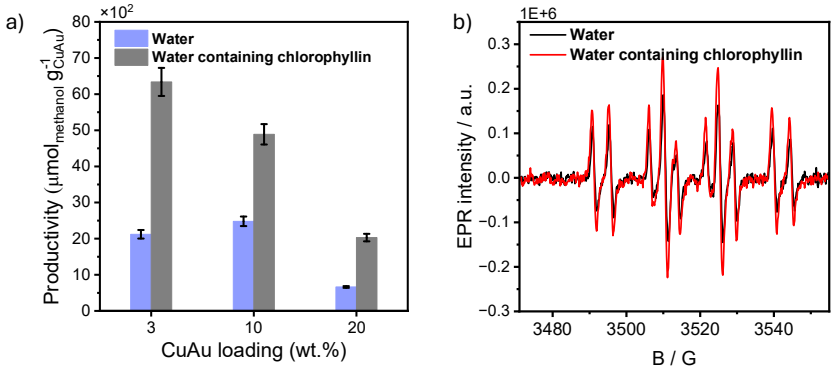

Fig 1. (a) Productivity to methanol formation (selectivity = 100%) in water and water containing 0.01 $g_{Chlorophyllin}$ L^{-1} at 160 °C/ 50 bar, **(b)** and operando EPR spectra in both mixtures, in the presence of DMPO in the presence of spin trap, respectively.

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EES - D2 - O06

CO_2 valorization via ionic liquids: A tandem process for the synthesis of cyclic carbonates and urethanes

Ramon Meseguer[1], Marina Pedrola[1], Adrianna Nogalska[1], Aitor Gual[1]
[1]*Eurecat, Centre Tecnològic de Catalunya, Unitat de Tecnologia Química, Tarragona, ES*

Growing concern over CO_2 emissions and the necessity for industrial decarbonization drive the research of efficient strategies for its valorization. CO_2 is an attractive C1 feedstock for synthesizing high-value compounds, such as cyclic carbonates and urethanes,[1] which are widely used as solvents, electrolytes, and polymer precursors.

Here, we describe a tandem procedure in which CO_2, propargylic alcohols and amines react convergently to form urethanes under mild conditions. First, the carboxylic cyclization of CO_2 and propargylic alcohols is carried out using imidazolium-based ionic liquids as both reaction medium and co-catalysts, with catalytic amounts of metal salts.[2] Under these conditions, the ionic liquid promotes CO_2 activation through *in situ* generation of an N-heterocyclic carbene,[3] which coordinates to the silver center to form the active catalytic complex.[4] This synergistic system enables the efficient activation of both CO_2 and the substrate, achieving high conversions and selectivity under moderate temperatures and pressures without volatile organic solvents. Subsequently, the intermediate cyclic carbonate undergoes nucleophilic ring-opening with primary or secondary amines to yield cyclic or acyclic urethanes. This 2-step approach constitutes a 3-component reaction in a one-pot tandem process, wherein the cyclic carbonate formed from CO_2 and propargylic alcohol reacts *in situ* with amines to yield the final product.[5]

Our results demonstrate that combining ionic liquids and metal catalysis constitutes a robust and versatile platform for chemical valorization of CO_2 under soft conditions. This methodology offers an advantageous alternative for transforming CO_2 into high-value products, confirming the potential of ionic liquids for cleaner and more energy-efficient chemical production.

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EES - D2 - O07

Liquid–solid phase separation-assisted direct CO_2 capture from air with a new system

Xiaopan Xue[1], Xuanbing Li[1], Soichi Kikkawa[1], Hideyuki Kawasok[1], Seiji Yamazoe[1]
[1]Graduate School of Science, Tokyo Metropolitan University, JP

Direct air capture (DAC) of CO_2 has attracted significant attention as an effective strategy to reduce atmospheric CO_2 levels.[1] In our previous studies, a liquid–solid phase separation system based on isophorone diamine (IPDA) and carbamic acid exhibited efficient CO_2 absorption at 400 ppm,[2] and aqueous solution of IPDA was shown to react with CO_2 at a 1:1 molar ratio when CO_2-containing gas was introduced by bubbling.[3] However, conventional bubbling processes suffer from pressure loss and sorbent vaporization, while solvent-based systems require excess energy for heating during CO_2 desorption.

To overcome these limitations, we developed a new system CO_2 absorption reactor that minimizes sorbent usage while maintaining high gas–liquid contact efficiency. Using this reactor, more than 90% of CO_2 (400 ppm) was continuously removed for 1153 min with 1.0 mmol of IPDA under H_2O vapor, achieving a total CO_2 uptake of 1.12 mmol. FT-IR analysis confirmed the coexistence of carbamic acid and bicarbonate species. In comparison, a conventional bubbling-type reactor using 1.0 mmol of IPDA and 1 mL of H_2O captured 1.00 mmol of CO_2 under identical conditions, indicating that the new system enables efficient CO_2 capture with reduced solvent usage. By contrast, neat IPDA under dry conditions showed lower performance, capturing only 0.64 mmol of CO_2, highlighting the critical role of H_2O vapor in reducing viscosity and enhancing gas–liquid contact. CO_2 desorption was achieved by treating the CO_2-loaded sorbent with methanol at 60 °C, following a reported procedure.[4] Confirming the effectiveness of the new system reactor for efficient and sustainable DAC.

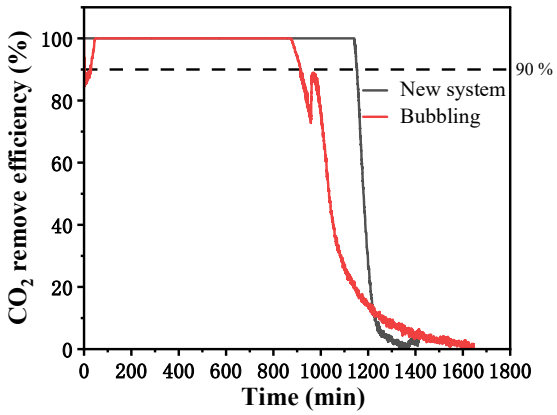

Fig. 1. CO_2 removal efficiency of IPDA evaluated using a bubbling-type reactor and a new system reactor. Absorption condition: IPDA, 1.0 mmol, 400 ppm CO_2, 50 mL/min. Temperature, ambient.

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EES - D2 - O08

From atmospheric deposition to photochemical transformation: Untargeted detection and phase-dependent fate of acetophenone in snow and water

Manuel Andino[1], Luca Carena[1], Elio Mondino[1], Davide Vione[1], Claudio Minero[1], Paola Calza[1]
[1]Dipto di Chimica, Università di Torino, IT

Snow environments are recognized as dynamic chemical matrices that influence the environmental fate of contaminants deposited from the atmosphere. In this study, we investigate the occurrence, sources, and photochemical fate of acetophenone (AcPh), a semi volatile aromatic compound, in alpine snow and surface water, with emphasis on the matrix-dependent processes.
AcPh was identified by untargeted UHPLC-HRMS analysis in all snow and water samples collected in the Monte Bianco area (northwestern Italian Alps), confirming its presence in remote high altitude environments. Semi-quantitative results revealed slightly higher AcPh signals at lower altitudes, suggesting the influence of regional emission sources. Backward air mass trajectory analysis indicated that long-range transport from industrialized and populated regions, combined with local valley recirculation, likely contributes to AcPh deposition in alpine snowpacks.
The photochemical fate of AcPh was investigated in artificial snow at 243 K and in liquid water under laboratory conditions, using different photosensitizers. The results showed that AcPh transformation is strongly matrix-dependent, with differences in reactivity and transformation pathways between artificial snow and liquid water. Additional experiments with real snow showed that the photochemical transformation of AcPh differs from that observed in artificial samples and in the melted phase. These findings indicate that snow is not merely a passive reservoir but an active medium that alters both the kinetics and pathways of contaminant transformation.
Overall, this work shows that the environmental fate of AcPh is controlled by its atmospheric origin and by strong phase-dependent effects, with snow playing a key role in controlling the persistence and transformation of AcPh in cold and remote regions.

Acknowledgements: This research was funded by the European Union under the Marie Skłodowska Curie Actions (MSCA) Doctoral Network IN2AQUAS (grant agreement No 101119555).

EES - D2 - O09
Air-soil exchange of PFAS – observations in rural central Europe and boreal forest

Gerhard Lammel[1,2], Karsten Baumann[1,3], Dominika Bezdeková[1], Jiři Kohoutek[1], Ondrej Letocha[1], Ludovic Mayer[1], Petra Přibylová[1], Roman Prokeš[1,4], Üllar Rannik[5], Petr Šenk[1], Risto Taipale[6]
[1]Masaryk University, Faculty of Science, RECETOX, Brno, CZ; [2]Max Planck Institute for Chemistry, Multiphase Chemistry Dept., Mainz, DE; [3]University of North Carolina, Gillings School for Global Public Health, Chapel Hill, USA; [4]Czech Academy of Sciences, Global Change Research Institute, Brno, CZ; [5]University of Helsinki, Department of Physics, Helsinki, FI; *[6]University of Helsinki, Institute for Atmospheric and Earth System Research, FI*

Per- and polyfluorinated alkyl substances (PFAS) are ubiquitous environmental pollutants[1-2], persistent, bioaccumulative, and toxic and a severe concern for ecosystems and human health[3-4]. Due to their semivolatile and surface active characteristics, their atmospheric fate and long-range transport potential is complex and poorly understood[5].
We determined the concentration of 12 perfluorocarboxylic (PFCAs), 5 sulfonic acids (PFSAs), 3 perfluoroalkane sulfonamides, 2 perfluoroalkylsulfonamidoethanols and 1 perfluoroalkylether carboxylic acid at a boreal forest (62°N) and a central European grassland (49°N) site. Air and soil samples were analysed using HPLC-MS/MS[6].
A much higher level of PFAS in air was found at the northern European site, 62-67 vs. 0.05-0.22 pg m^{-3}, dominated by perfluorobutanoic acid (PFBA) at both sites, while in soil the concentrations were comparable across sites i.e., 0.6-2.1 and 1.0-1.3 ng/g. The particulate mass fraction was minor, ≈1%.
Downward fluxes of air-soil exchange [7-8] were found for some PFSAs and PFCAs, while PFBA, PFHxA (both sites), PFHpA, perfluorooctanoic acid and perfluorooctane sulfonamide (central European site) were emitted from soils, during day and night.
These observations confirm the widespread distribution of PFAS in air and soil far from sources. Obviously, some PFCAs' long-range transport potential is enhanced by re-volatilisation, like previously found for chlorinated semivolatile organics[9].

Acknowledgements: Czech Science Foundation (17534S), Czech Ministry of Education, Youth and Sports (LM2023030, LM2023069, CZ.02.1.01/0.0/0.0/17_ 043/0009632).

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EES - D2 - O10

Comprehensive PFAS characterization in contaminated soils by integrated target, suspect, and non-target analysis combined with dTOP assay

Oliver Salangad[1], Francesca Cappelli[1], Anass Bouchikhi[1], Fabian Simon[1], Jodie Buytaert[2], Lieven Bervoets[2], Thimo Groffen[2], Adrian Covaci[1]

[1]Toxicological Centre, Department of Pharmaceutical Sciences, University of Antwerp, BE; [2]ECOSPHERE, Department of Biology, University of Antwerp, BE

Targeted analysis (TA) of per- and polyfluoroalkyl substances (PFAS), constrained by the limited availability of analytical standards, captures only a fraction of the total PFAS burden.[1,2] This leaves many emerging PFAS and precursors largely undetected. To address this gap, we combined TA, direct total oxidizable precursor (dTOP) assay, and high-resolution mass spectrometry (HRMS)-based suspect and nontarget screening (SS/NTS), for a comprehensive PFAS analysis in soils around a fluorochemical production (FCP) site in Flanders, Belgium.

Total soil PFAS concentrations around the hotspot reached 118 µg/g, among the highest worldwide.[3] SS/NTS reveals over 100 PFAS homologues and isomers across 14 classes, including pentafluorosulfide sulfonic acids (SF_5-PFSAs) and perfluorophosphoric diesters (PFPDEs). Furthermore, the optimized dTOP assay reveals distinct PFAS behaviours towards oxidation, such as the stability of short-chain (C4–C6) perfluoroalkyl sulfonic acids (PFSAs). Whereas longer PFSA homologues (C9–C15) exhibited partial degradation (28–97%), indicating susceptibility to chain shortening mechanisms. Similarly, long-chain perfluoroalkyl carboxylic acids (PFCAs ≥ C11) underwent sequential CF_2 elimination, consistent with stepwise oxidative shortening. Sulfonamide-based classes were fully degraded (> 99%), while perfluoroether carboxylic and sulfonic acids (PFECAs, PFESAs) displayed variable oxidation efficiencies. Emerging SF_5-PFSAs unexpectedly showed oxidation up to 95%. Transformation products, including nitrogen/sulfur containing intermediates, were also detected via diagnostic fragmentation data.

This integrated TA-SS/NTS-dTOP framework revealed previously unreported PFAS, transformation products, and precursors that extraction-based methods fail to detect. It also enables (semi-)quantitative precursor estimation and mechanistic interpretation of PFAS transformation, exposing the chemical complexity and source specificity of contamination at the FCP site.

Acknowledgements: We are grateful for the funding provided by the University of Antwerp and the Exposome Center of Excellence.

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EES - D2 - O11
From soil adsorption to bioavailability: Environmental fate of a plant-derived biostimulant

Michela Tramontini[1], Savarin Sinaviwat[2], Angwara Poolkasem[2], Paola Calza[1]
[1]University of Turin, IT; [2]Department of Science Service, TH

The widespread use of pesticides and fertilizers to meet global agricultural demands has raised concerns due to their persistence in the environment and potential accumulation in the food chain, leading to adverse ecological and human health effects. In response, biocompatible materials and plant-derived formulations are increasingly being explored as safer and more sustainable alternatives. In this study, the environmental fate of a novel commercial biostimulant based on plant-derived active substances was investigated in a representative Thai soil.
Soil characterization revealed a kaolinite-rich matrix with high bulk density and low cation exchange capacity, indicating limited adsorption sites and low permeability. Adsorption kinetics and equilibrium were examined through batch experiments, monitoring selected marker components of the biostimulant using ICP-MS and GC-MS. The results showed rapid adsorption, with more than 80% of the product immobilized within 30 minutes, and equilibrium achieved between 16 and 24 hours. Adsorption data were best described by a Langmuir isotherm, suggesting strong affinity for the clay matrix and preferential retention in surface soil layers. The pronounced immobilization implies high bioavailability in the rhizosphere and a strong potential for plant uptake. Accordingly, key bioactive properties of the biostimulant, including total phenolic content and antioxidant capacity, were assessed. The formulation exhibited a high phenolic content, which combined with its availability may contribute to reduced oxidative stress and enhanced plant immune responses. Overall, this work provided valuable insights into the environmental behaviour and agronomic potential of plant-derived biostimulant in tropical soil systems.

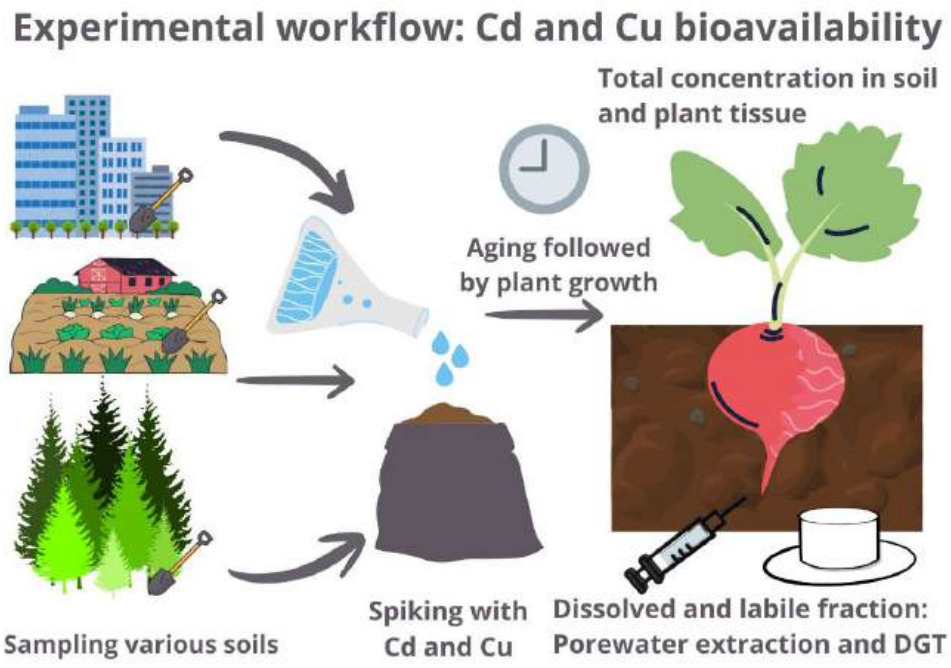
Acknowledgements: This work is supported by a PhD scholarship funded by the programme «Piano Nazionale Resistenza e Resilienza» (PNRR) of Next Generation EU and by the European Union's Horizon 2020 Research and Innovation Programme under the MSCA Grant Agreement No101007578 (SusWater).

EES - D2 O12
The influence of Cu and Cd additions on their bioavailability in uncontaminated soils

Delphine Vandeputte[1], Mateusz, Zawadzki[1], Lara Speijer[1], Marijke Huysmans[1], Marc Elskens[1], Willy Baeyens[1], Yue Gao[1]
[1]Vrije Universiteit Brussel, BE

Minor increases in trace metal concentrations in soil shift equilibria between solid phase and dissolved/labile pools, thereby altering bioavailability and plant uptake. In the environment, such small perturbations can be caused by for example application of fertilizers, traffic emissions, and atmospheric deposition. In this study, three uncontaminated Belgian soils with distinct origins (agricultural, urban, and forest) were spiked with half of the VLAREBO guidelines for Cd and Cu, keeping the total levels below/at these thresholds. Cadmium is highly mobile and toxic at all concentrations, whereas Cu, an essential element, binds strongly to organic matter and is only toxic at higher concentrations. After spiking, the soils were aged during which the dissolved and labile concentrations in porewater were regularly monitored until stabilization was observed. Diffusive Gradients in Thin films (DGT) passive samplers were applied to mimic root uptake and assess the labile pool. Over time, dissolved and DGT measured Cu in porewater decreased due to complexation with organic matter, whereas Cd concentrations increased due to a shift in chemical equilibrium reflecting the mobile character of this metal. After the aging, radish was planted in all soils and harvested. A total digestion of the plant material and soil indicated that Cu remained mainly bound to solid phase causing relatively small increases in plant concentrations, while Cd was less retained to soil and accumulated strongly in the plant tissue. Finally, a DGT time series deployment was carried out together with a porewater extraction to gain further insight into kinetics using the DGT Induced Fluxes in Sediments and Soils (DIFS) model. This study demonstrates that any potential perturbations in soil trace metal concentrations can strongly influence their bioavailability; contrasting behaviour of different metals across soils reveals insights not captured by total concentrations alone, highlighting the importance of studying speciation and lability in environmental settings.

This research is part of the GROW project in which experts from various fields and organisations work together to investigate safe reuse of wastewater in agriculture.



EES - D2 - O13
Dynamics of emerging PFAS in a contaminated terrestrial ecosystem

Oliver Salangad[1], Francesca Cappelli[1], Fabian Simon[1], Jodie Buytaert[2], Marcel Eens[3], Lieven Bervoets[2], Thimo Groffen[2], Adrian Covaci[1*]
[1]Toxicological Centre, University of Antwerp, BE; [2]ECOSPHERE, University of Antwerp, BE; [3]Behavioural Ecology and Ecophysiology Group, University of Antwerp, BE

Previous studies near a fluorochemical factory near Antwerp (Flanders) revealed the highest PFAS concentrations reported in soils, invertebrates, and songbird eggs. The main objective was to investigate the occurrence and fate of emerging PFAS in soil and their accumulation in songbird eggs.
Surface soil samples (n=30) were collected in 2024 close to the factory and were pooled into 7 composites. Eggs from great tits (Parus major) (n=29) and blue tits (Cyanistes caeruleus) (n=10) were collected from the same sites in April-May 2022. Suspect and non-target screening (SS/NTS) analyses were executed using LC-QTOF-MS, while LC-MS/MS quantified ~30 common PFAS.
In both soil and eggs, legacy PFAS classes were identified, such as sulfonates (PFSAs), including homologues (<C16) previously unreported. SS/NTS identified emerging PFASs, including pentafluorosulfide-perfluoroalkyl sulfonic acids (SF_5-PFSAs), ether-substituted carboxylic acids (PFECAs) and sulfonic acids (PFESAs). Certain homologues of SF_5-PFSAs (C6, C11), PFECA (C11–C12), and PFESA (C6–C9, C11, C13, C15) were present in eggs, but not in soil, suggesting biotransformation of SF5-PFSAs in birds to shorter homologues.
PFSAs were the major PFAS, comprising 24 % of total PFAS in soil and 86 % in eggs. PFOS was the most predominant, up to 1,000 ng/g in soil and 51,000 and 3,600 ng/g ww in great tit and blue tit eggs, respectively. Prevalence of FASAs (FOSA-2300 ng/g) and FASAAs (Et-FOSAA-7100 ng/g) was observed in soil. SF_5-PFSAs (3900 ng/g; 2% of total PFAS) were previously identified in soils impacted by AFFF. In great tit eggs, total SF_5-PFSAs reached up to 6200 ng/g, 5% of total PFAS. Among SF_5-PFSAs, the C9-homologue was the most predominant in both matrices, followed by the C8-homologue.
The soil and eggs showed overlaps, but also differences in contamination profiles and homologue distributions. SS/NTS approaches have the potential to identify overlooked PFAS to better understand and mitigate adverse effects.

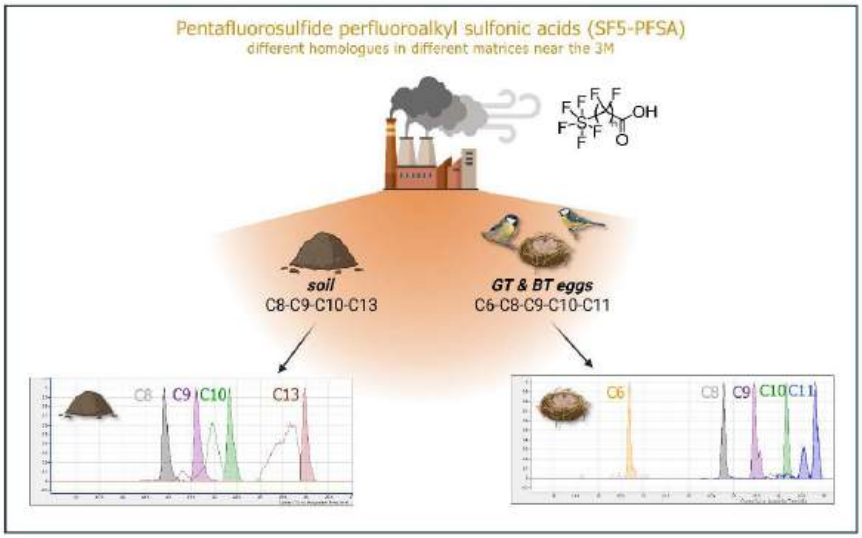


Fig. 1. Distribution of SF5-PFSAs homologues in soil and eggs samples.

EES - D2 - O14
Studying the synergistic effect between LDH and P25 for dyes removal from water

Christine Khoury[1], Sandra Adjeiwaa Ameyaw[1], Henri Knoth[1], Jennifer Strunk[1]
[1]*Technical University of Munich, DE*

The removal of dyes from water remained a significant environmental challenge. In this study, we investigate the synergistic effect between layered-double-hydroxides (LDH) and commercial TiO_2 P25 as hybrid materials for the removal of dyes. While LDH materials exhibit a strong affinity for the adsorption of dyes in their interlayer space, P25 is a well-studied photo-catalyst, limited by its wide band-gap, which restricts the light absorption to the UV region. Combining these two materials in one hybrid material is found to enhance both the adsorption mechanism and the photodegradation mechanism in the visible-light region, allowing to better utilize the solar spectrum.
LDH-P25 hybrid materials were prepared and systematically compared with the individual materials to distinguish adsorption, photocatalytic and synergistic effects. Dark adsorption experiments reveal enhanced dye uptake (>2 folds) in the presence of LDH-P25, compared with LDH alone. P25 alone has negligible dye uptake in dark, under the tested conditions. The photocatalytic tests under irradiation in the visible-light region demonstrate significant dye removal efficiency enhancement for the LDH-P25 hybrids. The observed performance of the LDH-P25 hybrids exceeds the sum of the individual components, indicating a synergistic effect between the LDH and P25 materials. This synergy is studied under in-situ DRIFTS experiments, which reveals significant shifts in the position and changes over time of peaks that are affected by light irradiation.

The authors would like to thank the TUM Global Postdoc Fellowship for funding this research.

EES - D2 - O15
Kraft lignin for efficient and sustainable mercury removal from aqueous systems

Bruno Henriques[1*], Ana Mendes[1], Inês Mendes[1], Nicole Ferreira[1,2], Thiago S.C. Silva[1], Thainara Viana[1], André M. da Costa Lopes[2,3], Eduarda Pereira[1]
[1]LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, PT; [2]CICECO, Dept. of Chemistry, University of Aveiro, PT; [3]CECOLAB, R. Nossa Senhora da Conceição, PT

Mercury (Hg) is one of the most critical contaminants due to its high toxicity and persistence[1]. It is particularly relevant in electronic waste (e-waste), where it is present in legacy components such as switches, lamps, and printed circuit boards[2]. Improper e-waste handling and processing for critical raw materials recovery, such as rare earth elements, can release Hg into aquatic environments and aqueous leachates, complicating separation processes and regulatory compliance, while existing treatment technologies remain costly or insufficiently selective.
Lignin is a low-value by-product of the pulp and paper industry, whose valorisation is central to circular economy strategies. This study evaluates the potential of Kraft lignin (KL) as a sustainable and low-cost sorbent for Hg removal from aqueous systems. Sorption performance was investigated over a wide range of initial Hg concentrations (25–1500 µg/L), in water matrices of different complexity (ultrapure and bottled mineral water), and under competitive conditions with other priority contaminants (As, Cd, Pb). Process optimisation was conducted using a Box–Behnken experimental design considering pH (4–8), sorbent dosage (20–200 mg/L), and initial Hg concentration (50–550 µg/L).
Sorbent dosage and initial Hg concentration were identified as the main factors influencing removal efficiency, while pH had a minor effect. Removal efficiencies up to 97 % were achieved within 6 h, reducing Hg concentrations to ~1 µg/L. Rapid kinetics were observed, and SIPS isotherm modelling indicated a maximum sorption capacity of 31,040 µg Hg/g KL. These results demonstrate the potential of Kraft lignin as a robust sorbent for Hg control in wastewater and e-waste leachates, contributing to safer and more sustainable processes.

This work is funded by COMPETE2030 FEDER 00847800. Thanks are due to UID/50006— Laboratório Associado para a Química Verde—Tecnologias e Processos Limpos and to PhD grants ref. 2022.13015.BD and 2022.13017.BD.

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EES - D2 - O16

Electrophilic additive–mediated chemical recycling of trithiocarbonate-terminated PMMA at high polymer concentrations

Jae-Won Lee[1], Young-Je Kwark[1]
[1]Dept. of Green Chemistry and Materials Engineering, Soongsil University, KP

Plastic waste management requires sustainable recycling routes beyond mechanical processes that often downcycle materials. Chemical recycling via depolymerization can enable closed-loop use by regenerating monomers, yet vinyl polymers are difficult to depolymerize because conversion of σ-bonded backbones to π-bonded monomers is thermodynamically disfavored, typically demanding harsh conditions. Here, we develop a mild depolymerization strategy for trithiocarbonate-terminated poly(methyl methacrylate) (PMMA) at high polymer concentration using electrophilic additives—fluorinated alcohols and triflate salts. Fluorinated alcohols act as strong hydrogen-bond donors due to the inductive effects of fluorine substituents, while triflate salts can provide Lewis-acidic centers that interact strongly with the electron-rich carbonyl groups of PMMA. These interactions modulate the local steric/electronic environment, promote depropagation, and alter the behavior of depropagating radicals to suppress side reactions during depolymerization. Hydrogen-bonding interactions were examined by ^{1}H-NMR, including variable-temperature measurements to track temperature-dependent changes, as well as in situ Raman spectroscopy. In addition, depropagating methyl methacrylate (MMA) radicals were probed by electron paramagnetic resonance under varied additive structures and concentrations. Depolymerization performance was assessed by monomer conversion using quantitative NMR and gas chromatography (GC). Overall, this work demonstrates successful recovery of high-purity MMA monomer under mild, high-concentration conditions and provides mechanistic insights for sustainable chemical recycling of vinyl polymers.

EES - D2 - O16

Assessment of CO_2 quality across capture, liquefaction, and storage in a cement CCS pilot plant

Ward Peeters[1], Randi Neerup[1], Maria Dimitriadi[1], István Györbiró[1], Mads F. Hennings[1], Rasmus K. Engilbertsson[1], Søren Jensen[2], Jakob L. Karlsson[2], Quynh Thu Nguyen[3], Betina Jørgensen[4], Halil Halilov[5], Philip L. Fosbøl[1]

[1]Technical University of Denmark (DTU), Dept. of Chemical Engineering, Center for Energy Resources Engineering (CERE) DK; [2]Pentair Union Engineering A/S, DK; [3]Danish Technological Institut, DK; [4]Evida Service A/S, DK; [5]Aalborg Portland A/S, DK

Carbon capture and storage (CCS) is a key technology for reducing CO_2 emissions from the cement industry[1]. While extensive research has focused on capture performance, significantly less experimental evidence is available on the quality of cement-derived CO_2 across the downstream CCS value chain. Impurities originating from flue gas may affect CO_2 liquefaction, transport, storage, and utilization, highlighting the need for pilot-scale data under realistic operating conditions.

This work presents an integrated assessment of CO_2 quality across capture, liquefaction, and storage at a pilot-scale CCS facility connected to a cement plant in Aalborg, Denmark. During an operational campaign in 2025–2026, CO_2 is captured from cement kiln flue gas using the CESAR1 solvent, a blend of 2-amino-2-methyl-1-propanol (AMP) and piperazine (PZ), and subsequently conditioned, liquefied, and stored on site. The CO_2 liquefaction unit and storage setup are shown in **Fig. *1***.

Fig. 1. A) CO_2 liquefaction unit, and B) CO_2 storage tank at Aalborg Portland

CO_2 quality is monitored continuously using an online gas-phase Fourier Transform Infrared (FTIR) analyser, enabling detection of a broad range of gaseous impurities and water content at low concentrations. Measurements are performed at three locations along the process chain: upstream of liquefaction, downstream of liquefaction, and after storage in a liquid CO_2 tank.

Initial results show that small concentrations of impurities are present in the captured CO_2 prior to liquefaction. These impurities decrease to below detection limits after passing through the liquefaction unit, likely due to dehydration and adsorption steps in the conditioning process. Furthermore, medium-term monitoring of liquid CO_2 storage shows no observable accumulation of impurities, indicating stable CO_2 composition during storage under the investigated conditions.

Overall, this study provides pilot-scale evidence that CO_2 captured from cement flue gas can be effectively conditioned to meet downstream CCS quality requirements, emphasizing the importance of post-capture conditioning and multi-point CO_2 quality monitoring.

Acknowledgements: The authors would like to acknowledge funding provided from the CASPER project, funded by INNO-CCUS (pool 2 no. 1-P8), and the support of the Technical University of Denmark (DTU).

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EES - D2 - F01
Shining light on plasma catalysis: Transparent DBD reactors for CO_2 conversion

Christine Vantomme[1,2,3], Sammy Verbruggen[1,2], Annemie Bogaerts[3]
[1]Antwerp engineering, photoelectrochemistry and sensing (A-PECS), University of Antwerp, BE; [2]NANOlight Center of Excellence, University of Antwerp, BE; [3]Plasma Lab for Applications in Sustainability and Medicine – Antwerp (PLASMANT) and PLASMA Center of Excellence, University of Antwerp, BE

Carbon Capture and Utilization (CCU) is a key strategy to mitigate excessive atmospheric carbon dioxide (CO_2) levels, by capturing and converting CO_2 into value-added products. Among emerging CCU technologies, plasma catalysis is particularly promising. It employs a reactive chemical cocktail -generated by plasma, driven by electrical energy - in combination with a catalyst to enhance process selectivity and exploit synergistic plasma–catalyst interactions.[1] Despite its potential, significant challenges remain, notably the development of catalyst materials optimized for plasma environments and plasma reactor designs that ensure improved plasma–catalyst contact.[2] In this study, we investigate the integration of plasma with a semiconductor catalyst (photocatalyst) and an external UV light source, to perform plasma-photocatalysis (Fig. 1). A novel, custom-made transparent dielectric barrier discharge (DBD) reactor was designed as a starting point. Multiple reactor configurations were systematically compared. Three electrode materials were investigated: stainless-steel mesh, indium-doped tin oxide (ITO)-coated quartz, and fluorine-doped tin oxide (FTO)-coated glass (Fig. 2). In addition, a double DBD (DDBD) configuration was explored by introducing a borosilicate plate into the discharge gap. The potential of a surface DBD (SDBD), consisting of an Al_2O_3 dielectric plate with Ni-coated metal grid electrodes, screen-printed on the surface, was also evaluated. SDBD configurations are particularly attractive as they can generate a more uniform plasma and improve plasma-catalyst surface interaction.[2] All reactor configurations were benchmarked for pure plasma CO_2 splitting in terms of CO_2 conversion, plasma power, energy efficiency, UV-light transparency, and electrode lifetime. The detailed experimental setup and key results will be presented.

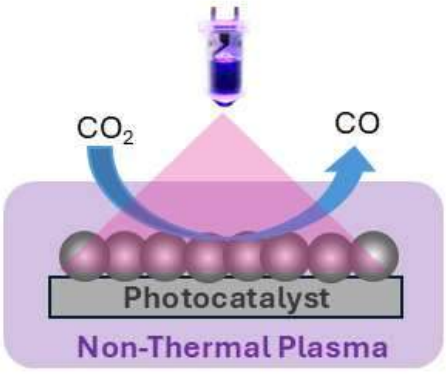

Fig 1. Concept of plasma-photocatalysis

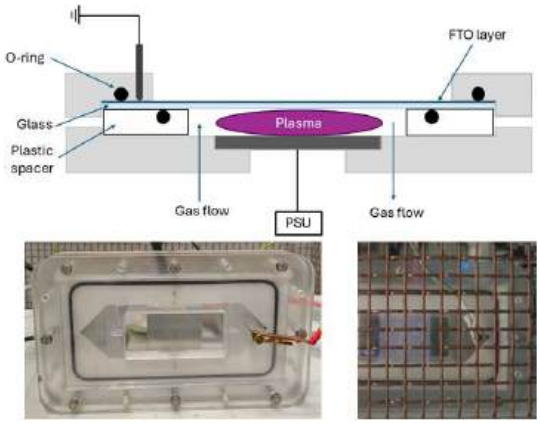

Fig 2. Schematic (up) and pictures (below) of the reactor configuration.
Plasma off (left) plasma on (right)

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EES - D2 - F02
Towards greener energy: Bio-based alternatives for sodium-ion battery components

Renata Matos[1], Mónica Marques[1], Rita Carvalho Veloso[1]
[1]*Vasco da Gama CoLAB – Energy Storage, PT*

The accentuated population growth, increase in energy consumption and environmental concerns are boosting the development of sustainable energy storage devices. Electrochemical storage systems are considered a good option to meet global energy demands, as proven by the popularity of lithium-ion batteries (LIBs) over the last decades in the electric vehicles and consumer electronics industries. However, LIBs present significant limitations, including lithium natural scarcity, high production cost and safety issues.[1]
Sodium-ion batteries (SIBs) have emerged as a sustainable alternative for LIBs, mainly due to the high abundance and global distribution of sodium, which leads to lower production costs and mitigates geopolitical tensions, and higher safety.[2] Moreover, as SIBs are very similar to LIBs, operating on basis of intercalation chemistry, existing production lines of LIBs can be easily adapted to obtain SIBs.[1] Nevertheless, SIBs commercialization is dependent on increasing its energy densities to values competitive to LIBs. As so, the optimization of SIBs cathodes and anodes has been a major research focus, always considering both scalability and sustainability factors.[2]
Herein, we discuss several strategies to prepare cost-effective and sustainable anodes for SIBs, focusing on the replacement of conventional PFAs-based binders to bio-based alternatives (such as carboxymethyl cellulose) and the development of biomass-derived active materials. Furthermore, to lower the environmental impact and the production cost, our anodes were prepared in a water/isopropanol system in alternative to the conventionally used toxic solvents (e.g. NMP).

This work was financially supported by PRR project 01/C05-i02/2022.P269 – “Missão Interface”, funded by the Recovery and Resilience Plan (Plano de Recuperação e Resiliência – PRR) of the Portuguese Republic, under the NextGenerationEU framework.

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EES - D2 - F03

Rapid combustive mechanochemical synthesis of metal chalcogenides for energy conversion applications

Matej Baláž[1], Imelda Octa Tampubolon[1,2], Magdaléna Strečková[3], Saba Sepahban Shahgoli[4,5], Umut Aydemir[6]

[1]Institute of Geotechnics, Slovak Academy of Sciences, SK; [2]Faculty of Materials, Metallurgy and Recycling, Technical University of Košice, SK; [3]Institute of Materials Research, Slovak Academy of Sciences, SK; [4]Koç University Boron and Advanced Materials Application and Research Center (KUBAM), TR; [5]Graduate School of Sciences and Engineering, Koç University, TR; [6]Department of Chemistry, Koç University, TR

Mechanochemistry is currently seeing a peak of its utilization for organic reactions and soft syntheses not requiring a lot of energy.[1] However, it has been around also for the inorganic synthesis even for longer time.[2] In this contribution, the utilization of a high-energy ball milling for a combustive synthesis of metal chalcogenides will be demonstrated. This reaction pathway offers faster and energy-saving alternative to the traditional gradual mechanochemical reactions.[3] This will be demonstrated for copper and nickel sulphides. In both cases, the reaction can be completed within few seconds[3,4] (Fig. 1) and for the Cu-S system, the presence of milling balls is even not necessary.[5] In the end, the applicability of the prepared copper and nickel sulphide for waste heat into electricity conversion (thermoelectrics) and for hydrogen generation via water splitting (electrocatalysis) will be shown.

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-24-0353.

Fig. 1. Rapid mechanochemical synthesis of copper and nickel sulfides for energy conversion applications

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EES - D2 - F04

Pt-Ru based nanomaterials enabling coupled cathodic hydrogen evolution and anodic formaldehyde oxidation in fuel cell systems

João Pedro da Silva Jaques[1], Ahmad Tayyebi[1], María Giménez López[1]
[1]Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), ES

In the context of the energy transition, hydrogen has recently attracted increasing interest as a key energy carrier. The need for efficient catalysts for water electrolysis has driven the search for alternatives capable of operating effectively in alkaline media, where conventional platinum-based catalysts exhibit reduced activity. In this work, a platinum (Pt)-based electrocatalyst modified with ruthenium (Ru) is developed for the hydrogen evolution reaction (HER) in both alkaline and acidic electrolytes. While Pt exhibits excellent catalytic performance in acidic media, its activity in alkaline environments is limited by sluggish water dissociation kinetics. In contrast, Ru, a relatively more abundant and cost-effective noble metal, displays high intrinsic activity for water activation. By combining the complementary properties of both metals, the proposed catalyst aims to enhance HER performance across a wide pH range[1].

The synthesized nanostructures exhibit improved HER activity in both electrolytes, with lower overpotentials and accelerated reaction kinetics compared to commercial reference catalysts. These results indicate a strong synergistic interaction between Pt and Ru (**figure 1**), consistent with enhanced water dissociation and optimized hydrogen adsorption. Beyond conventional water electrolysis, this work also explores the integration of these materials into hybrid electrochemical energy conversion systems. In this concept, the Pt-Ru catalyst is envisioned as the cathodic material for hydrogen evolution reaction, while the anodic reaction involves the formaldehyde oxidation reaction, enabling simultaneous hydrogen generation and chemical upgrading within a fuel cell-type architecture[2].

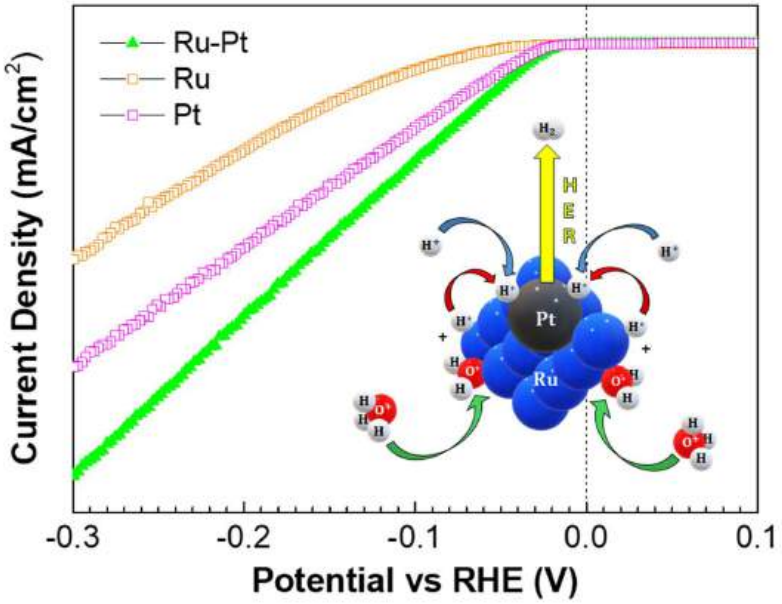

Fig. 1. Polarization curves of Pt-Ru catalysts in acidic electrolytes compared with reference materials and schematic illustration of the synergistic HER mechanism.

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EES - D2 - F05
Enhancing photosynthetic light utilisation with wavelength-shifting polymer films

Lan Nan[1], Norbert J. Janowicz[1], Chao Bao[1], Erwin Reisner[1], Dominic S. Wright[1,*], Jenny Zhang[1,*]
[1]*Yusuf Hamied Department of Chemistry, University of Cambridge, UK*

Natural photosynthesis is limited by incomplete absorption of the solar spectrum, particularly in the ultraviolet (UV) region, where light is both underutilized and damaging to photosynthetic organisms.[1] This spectral mismatch constrains both energy fixation efficiency and the long-term stability of photosynthetic systems. Although extensive research has investigated the use of light down-shifting (LDS) materials in horticultural applications, relatively few studies have successfully translated this approach to photobioreactors, which offer superior scalability and biomass productivity compared with horticulture.[2,3] Here, we present a simple and modular light-management strategy that extends photosynthetic light utilization into the UV range through the use of LDS polymer films.

Europium complexes were incorporated into a PMMA substrate via solution casting to fabricate optically tunable LDS films capable of converting UV radiation into red emission. The films were placed externally on bioreactor tanks containing cyanobacteria, enabling non-invasive spectral modification of incident light. Under UV illumination, the LDS films increased short-term photosynthetic oxygen evolution by up to threefold relative to control conditions. In addition, enhanced photocurrent generation was observed in a mediated three-electrode electrochemical system, confirming improved photochemical activity. Beyond short-term performance, the LDS films also mitigated UV-induced photodamage and promoted sustained cyanobacterial growth during prolonged UV exposure in bioreactor environments.

This work demonstrates that spectral down-shifting provides an effective route to harness otherwise detrimental UV light for productive photosynthesis while simultaneously protecting biological systems. Importantly, our findings highlight that optimal LDS film performance arises from the synergistic interplay of spectral conversion efficiency, optical haze, and surface morphology. These insights establish a design framework for next-generation LDS materials aimed at maximizing light penetration and utilization in photosynthetic and biohybrid energy systems.

Acknowledgement: The work was funded by the Leverhulme Trust Research Project Grant RPG-2024-309. Thank you to Lambda Energy (trading Lambda Agri) for providing additive and film samples for comparative studies with industry standard in this work.

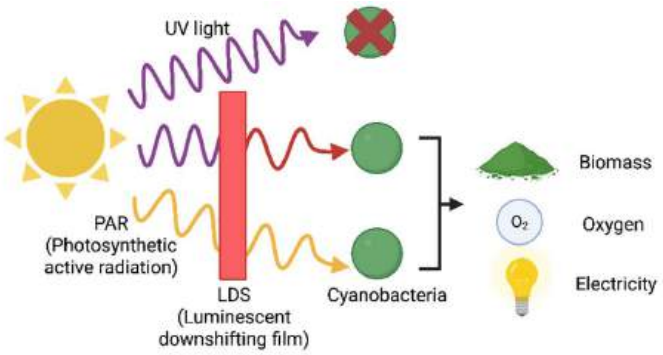

Fig. 1. Schematic representation of the application of luminescent downshifting film (LDS) for model photosynthetic system – cyanobacteria.

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EES - D2 - F08
New insights in the tricky reaction of isopropanol dehydration to propylene

Georgeta Postole[1], Tristan Cabanis[1], Tien-Hoang Nguyen[1], Aline Auroux[1], Jean-Luc Dubois[2]
[1]Université Claude Bernard Lyon, FR; [2]Trinseo Netherlands B.V., NL

The worldwide increasing demand for propylene [1,2] and its shortage due to the shale gas revolution and environmental challenges requires alternative, economically viable, and sustainable pathways of production.
In this study, commercial alumina and silica–alumina catalysts (cost-effective materials that can be used for application at industrial scale) are investigated for propylene production via isopropanol dehydration reaction. Isopropanol is an appropriate feedstock for small on-site production and for providing on-demand a large panel of compounds therefore avoiding transportation and storage [3]. Isopropanol dehydration to propylene is not new to the catalysis world but the formation of side products makes it still a tricky reaction that requires very fine catalysts tuning (specific acidity and porosity, good stability, resistance to steam and high activity) for attaining polymer grade propylene.
The textural properties, structure and chemical composition were determined for as-received and hydrothermally treated catalysts. The nature, amount, and strength distribution of acid–base sites were determined by adsorption microcalorimetry and FTIR. The reaction conditions (200 – 300 °C, $P_{isopropanol}$ = 5136 Pa) were chosen to fit with a further propylene conversion into value-added compounds (e.g. acrolein) with minimal capital cost.
It was found that surface area, pore-size distribution and pore volume are not determining factors for the catalytic performances. The best-performing catalyst combined stable textural properties and a large number of high-strength acid sites under hydrothermal conditions (Fig. 1).
The importance of determining the acid properties of water-aged catalysts, when considering reactions where water is present as reactive or product, will be discussed.The activity data obtained in a pulse flow reactor, using coupled calorimetry-chromatography and DRIFT-MS will be compared with the results in continuous flow. Studying the reaction inside a differential scanning calorimeter linked to a GC allowed to differentiate and measure the adsorption/desorption/reaction (exothermic/endothermic) heats occurring at the catalyst surface.

Funding: This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 101037009.

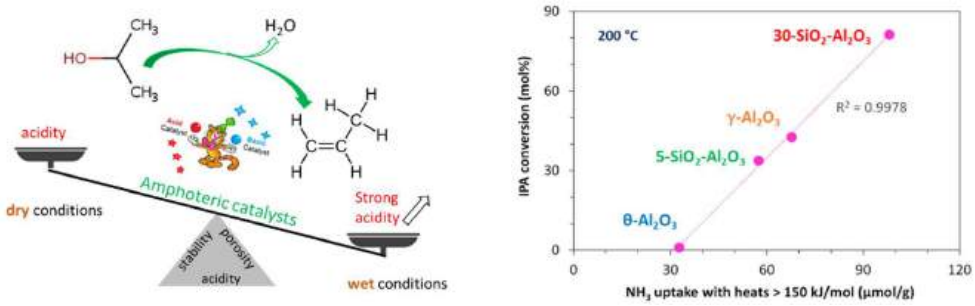

Fig. 1. Correlation between the number of strong acid sites of water-aged catalysts and IPA conversion

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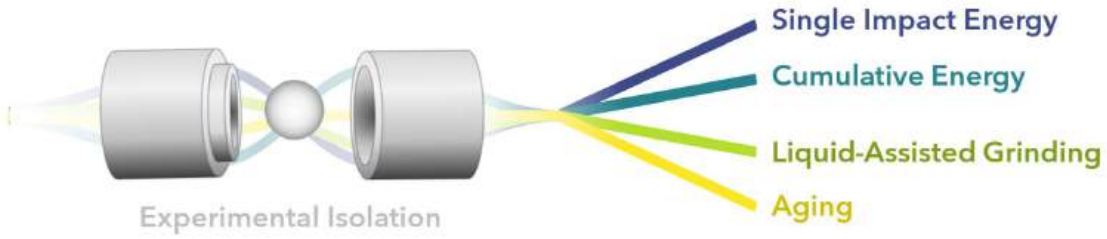
EES - D2 - F09

Decoding mechanochemical drivers: Experimental isolation of single impact, cumulative energy, aging and liquid-assisted grinding effects in organic mechanosynthesis

Johanna Templ[1], Lars Borchardt[2]
[1]TU Wien, Institute of Applied Synthetic Chemistry, AT; [2]Ruhr-Universität Bochum, DE

Mechanochemistry is rapidly transitioning from a green alternative to a powerful tool in organic synthesis.[1] Yet, the persistent “black box” nature of ball milling, where kinetic energy is often treated as an empirical variable, limits its predictive use. To move from trial-and-error toward guided synthesis, a deeper understanding of how mechanical force triggers organic transformations is essential.[2]



We demonstrate an experimental approach to isolate the individual drivers of mechanochemical reactivity.[3] Using a standardized mixer mill setup, we disentangle the roles of single-impact energy (E_{impact}), cumulative energy (E_{total}), liquid-assisted grinding (LAG), and secondary effects. By investigating two distinct all-solid reactions, the Wittig olefination[4] and the Finkelstein halogen exchange, we reveal a fundamental duality in mechanochemical pathways. The Wittig reaction behaves as an *impact-complete* system: conversion occurs exclusively during active milling and scales linearly with E_{total}, making it a robust benchmark for energy scaling across milling devices. In contrast, the Finkelstein reaction is *impact-triggered*, where mechanical force initiates a process that continues through post-impact aging. Rather than treating aging as an uncontrolled process, we quantify how its rate and extent correlate with E_{impact}, enabling high conversions with reduced overall energy input. Finally, we address the question of whether LAG-enhanced diffusion outweighs the role of impact energy. Our results prove that LAG does not replace the impact-driven regime but modulates it by balancing energy transfer with enhanced diffusion, clarifying the elusive LAG *sweet spot*. By isolating and quantifying these mechanochemical drivers, we provide a framework for controlled and reproducible organic mechanosynthesis, shifting the field toward guided control of mechanochemical transformations.

This work was funded by the Austrian Science Fund (FWF), grant number: 10.55776/J4922.

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EES - D3 - O01

Control of electrocatalytic levulinic acid valorization: Synergistic tuning of catalysts, solvents, and temperature

Pol Vilariño[1,2], Elvira Gómez[1,2], Albert Serrà[1,2]
[1]Grup d'Electrodeposició de Capes Primes i Nanoestructures (GE-CPN), Departament de Ciència de Materials i Química Física, Universitat de Barcelona, ES; [2]Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Barcelona, ES

Electrocatalytic hydrogenation (ECH) of levulinic acid (LA) has emerged as a highly versatile and sustainable platform for converting biomass-derived feedstocks into value-added chemicals such as γ-valerolactone (GVL), valeric acid (VA), and 4-hydroxyvaleric acid (HVA). Recent advances demonstrate that the overall efficiency, selectivity, and energy requirements of this transformation are governed by the interplay between catalyst architecture, reaction medium, and temperature. [1,2]

Studies across aqueous and organic solvents reveal that properties such as viscosity, polarity, ionic conductivity, and solvation strongly influence mass transport, proton availability, intermediate stability, and hydrogenation kinetics. These effects enable high LA conversions and GVL selectivity's above 90% when using nickel-based electrocatalysts under optimized solvent conditions.

Parallel progress in catalyst design has further expanded the capabilities of ECH. Electrodeposited mono-, bi-, and trimetallic Cu, Ni, and Ru systems show enhanced faradaic efficiencies, activity, and long-term stability. Ni-rich compositions, particularly in binary and ternary configurations, yield LA conversions above 85% and high GVL selectivity in acidic media, while alkaline environments shift the process toward VA formation with lower overall performance. These catalysts also exhibit minimal degradation and very low metal leaching, highlighting their suitability for scalable and cost-effective electrochemical upgrading.

Temperature has recently been identified as a decisive switch for directing the LA reduction pathway. Low temperatures selectively promote HVA formation, whereas moderate temperatures drive efficient lactonization toward GVL with near-quantitative yields. Nanostructured electrodes such as vertically aligned graphene-based supports further magnify this tunability by improving hydrogen activation and surface transport, resulting in significantly reduced energy consumption.

Together, these insights establish a unified framework in which solvent environment, catalyst composition, and temperature can be jointly tuned to precisely steer the reaction network. This integrated approach positions ECH as a flexible, energy-efficient, and environmentally friendly strategy for the selective electrochemical valorization of renewable biomass resources.

Acknowledgements: Grant CNS2024-154690 funded by MICIU/AEI/10.13039/501100011033 and, as appropriate, by "ESF Investing in your future", by "ESF+" or by "European Union NextGenerationEU/PRTR". The authors also would like to express their gratitude to the Departament de Recerca i Universitats, particularly the Departament d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR) for their support. Authors thank the CCiT-UB for the use of their equipment.

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EES - D3 - O02

Influence of catalyst composition and temperature on glycerol electrooxidation in continuous-flow electrolysis

Martí Molera[1,2], Angel Cuesta-Ciscar[3,4], Teresa Andreu[1]

[1]Sustainable Electrochemical Processes (SEP). Departament de Ciència dels Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona (UB), ES; [2]Departament d'Enginyeria Electrònica i Biomèdica. Universitat de Barcelona (UB), ES; [3]Advanced Centre for Energy and Sustainability (ACES), School of Natural and Computing Sciences, University of Aberdeen, UK; [4]Instituto de Química Física Blas Cabrera, ES

The electrooxidation of glycerol presents a dual opportunity for sustainable chemistry: upgrading a biodiesel byproduct and reducing the energetic cost of hydrogen by replacing the oxygen evolution reaction. However, the complexity of glycerol oxidation requires the careful selection of electrocatalyst materials and operating conditions to enable both activity and product selectivity. In this work, we investigate the influence of catalyst composition, temperature, and flow conditions on glycerol electrooxidation using three representative electrocatalysts supported on nickel foams: a first-row transition-metal NiCo oxide, a noble-metal AuIn alloy, and a hybrid PdNi alloy.

Electrochemical characterization combined with in-situ UV–vis reflectance spectroscopy reveals catalyst-dependent oxidation mechanisms. The NiCo oxide follows an oxyhydroxide-mediated pathway that favours high selectivity toward formic acid. In contrast, the AuIn alloy operates through an adsorbed hydroxide-mediated mechanism, promoting the formation of C_3 products such as glyceric acid and dihydroxyacetone. The PdNi alloy displays a dual mechanism, with its selectivity shifting according to its oxidation state. Reflectance measurements further demonstrate that, on noble and hybrid catalysts, glycerol consumption delays surface oxidation by depleting adsorbed hydroxide species, preserving the metallic state and preventing catalytic inhibition.

Continuous-flow electrolysis experiments conducted at 25, 40, and 60 °C and different flow rates reveal that temperature is a key operational parameter. Elevated temperatures enhance reaction kinetics, lower cell potential, and mitigate catalyst passivation by accelerating surface reactivation. Flow rate additionally modulates selectivity by tuning reactant residence time, with higher flow favouring intermediate oxidation products.

Overall, this study establishes clear mechanistic correlations between catalyst composition, operating temperature, and product distribution. These insights provide guidelines for designing efficient continuous-flow systems for glycerol valorization and advancing energy-efficient electrolysers.

This work was supported by the Ministerio de Ciencia e Innovación and FEDER-UE [PID2022–138491OB-C33 (MICIU/AEI/10.13039/501100011033)]; AGAUR Generalitat de Catalunya [2024 FI-1 00421].

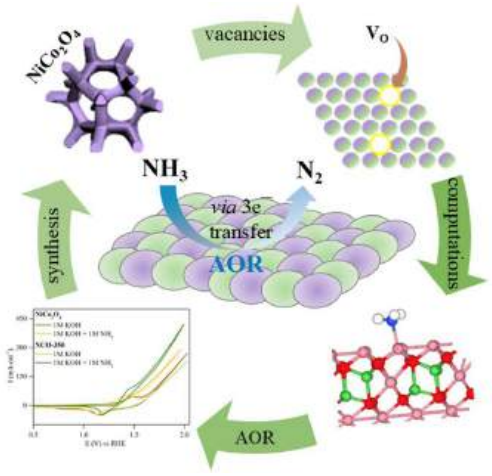
EES - D3 - O03

Oxygen defected NiCo spinel structures for ammonia electrooxidation reaction: An experimental and theoretical approach

Justyna Luczak[1], Sara Sumbal[1], Adrian Olejnik[2], Marek Lieder[3]

[1]Dept. of Process Engineering and Chemical Technology, Faculty of Chemistry, Gdansk University of Technology, PL; [2]Dept. of Metrology and Optoelectronics, Faculty of Electronics, Telecommunications, and Electronics, Gdansk University of Technology, PL

Designing highly selective, stable, and economical catalysts for the ammonia electrooxidation reaction (AOR) is crucial to improve the electrochemical energy conversion and storage technologies[1]. Hereby, we disclose oxygen-defected NiCo-based spinel structures, obtained by direct deposition of spinel on Ni foam and subsequent thermal treatment under Ar/H_2 atmosphere, as efficient electrocatalysts for AOR. The electrocatalytic surface area values (ECSA) for $NiCo_2O_4$ and defective samples were higher than the sum of the ECSA values of NiO and Co_3O_4. This indicates more active surface area for AOR due to combining Ni and Co oxides in the spinel structure, which contributes to enhanced catalytic activity. Among the prepared electrocatalysts, NCO-350 was found to exhibit the highest AOR activity with regard to current density (125 $mA{\cdot}cm^{-2}$) as well as turnover frequency (1.46 s^{-1}). The N_2 selectivity at 1.55 V *vs* RHE was more than 81 %, whereas ammonia oxidation efficiency was 93 % upon completion of the 120h stability test. Theoretical calculations revealed that the exposure of the electrocatalysts to the Ar/H_2 atmosphere induces two types of defects: oxygen vacancies and H-atoms built into the crystal. The density of states (DOS) spectra confirmed the higher DOS for $NiCo_2O_4$ at the Fermi level as compared to the constituent single-oxides[2].



This work was funded by OPUS program of the National Science Centre, Poland (UMO-2021/41/B/ST4/03255). A.O. would like to acknowledge the support of Foundation of Polish Science (FNP) with scholarship START 062/2025.

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EES - D3 - O04
Modelling metal electrocatalysts as cathodes: The urgent need to look beneath the surface

Matthias Vandichel[1]*, Raju Lipin[1], Muhammad Umer[1], Sousa Javan Nikkhah[1]
[1]*University of Limerick, IE*

DFT-based simulations are indispensable for probing nano catalyst behavior at the atomic level. By resolving each elementary step, they disentangle competing pathways, establish quantitative structure–activity relationships and guide the rational design of novel electrocatalysts. However, when applied to electrochemical systems, DFT models must also account for variables such as electrode potential, pH, temperature, adsorbate partial pressures, and surface structure. These factors collectively dictate whether chemical species adsorb, absorb into the subsurface, or incorporate into the lattice, driving nanomaterial behavior that far exceeds "simple" surface chemistry. In this talk, an overview will be given of how subsurface hydrogen affects the surface structure of the active sites. We will also discuss how the hydrogen evolution reaction pathways for Pd-based electrocatalysts are altered and provide a future outlook on the description of electrocatalysts.[1-7]

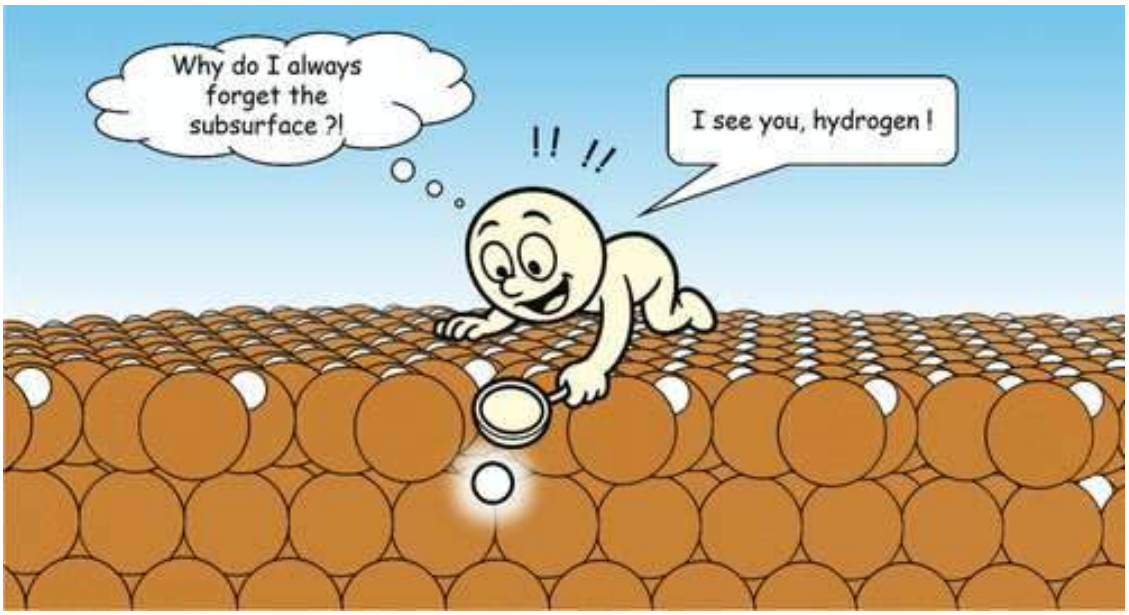

Fig. 1. Cartoon illustration highlighting the often-overlooked role of subsurface hydrogen in modelling metal electrocatalysts.

Acknowledgments: M.V. acknowledges funding from Research Ireland under the Frontiers for the Future Programme (MEM-E-TECH, 23/FFP-A/12221) and from the Horizon Europe research and innovation programme (SUN2CN, Grant Agreement No. 101223193). The authors acknowledge the Irish Centre for High-End Computing (ICHEC) for providing computational facilities and support.

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EES - D3 - O05

Enhancing performance of electrochemical reactors through pulsatile electrolyte flow and 3D-printed electrodes

Kavin Teenakul[1], Jonas Hereijgers[1]
[1]Research Group Applied Electrochemistry & Catalysis, University of Antwerp, BE

Enhancing the performance of electrochemical reactors such as flow batteries and electrosynthesis cells can be achieved by increasing mass transport inside the cell. Pulsatile flow has been shown to increase mass transport by up to a factor of 1.93 on a flat electrode with a plastic turbulence promoter. However, a flat electrode has a low surface area, restricting the maximum power the cell can operate at[1]. Another study increased flow battery capacity by 39% using pulsatile flow with a felt electrode[2]. Felt electrodes provide high surface area yet suffer from high pressure drops and dead zones, increasing pumping power. A promising approach to increase surface area while reducing pressure drop is the incorporation of 3D-printed electrodes, which offers flexibility to tune electrode geometry and porosity[3]. Despite these advances, a critical gap in the literature remains, as the combined effects of pulsatile flow and 3D-printed electrodes on mass transport and pumping power have not been systematically investigated. Addressing this gap is essential for assessing the application of pulsatile flow in electrochemical reactors.
In this work, the effects of electrolyte flow rate, frequency, and pulse amplitude on mass transport and pumping power of various 3D-printed electrode structures were studied. Limiting current was measured to calculate the volumetric mass transport coefficient using the electrochemical copper deposition reaction. Pumping power was determined from measured pressure drop and flow rate. The results show that the volumetric mass transport of pulsatile flow exceeds that of steady-state flow at an electrolyte pumping power of 19 W/m³ for a body-centered cubic lattice electrode design. Additionally, conversion reaches 16% compared to 10% for steady-state flow at a net flow velocity of 0.35 cm/s. In conclusion, pulsatile flow combined with 3D printed electrodes increases mass transport and conversion at lower pumping power, highlighting its potential to improve electrochemical reactor performance.

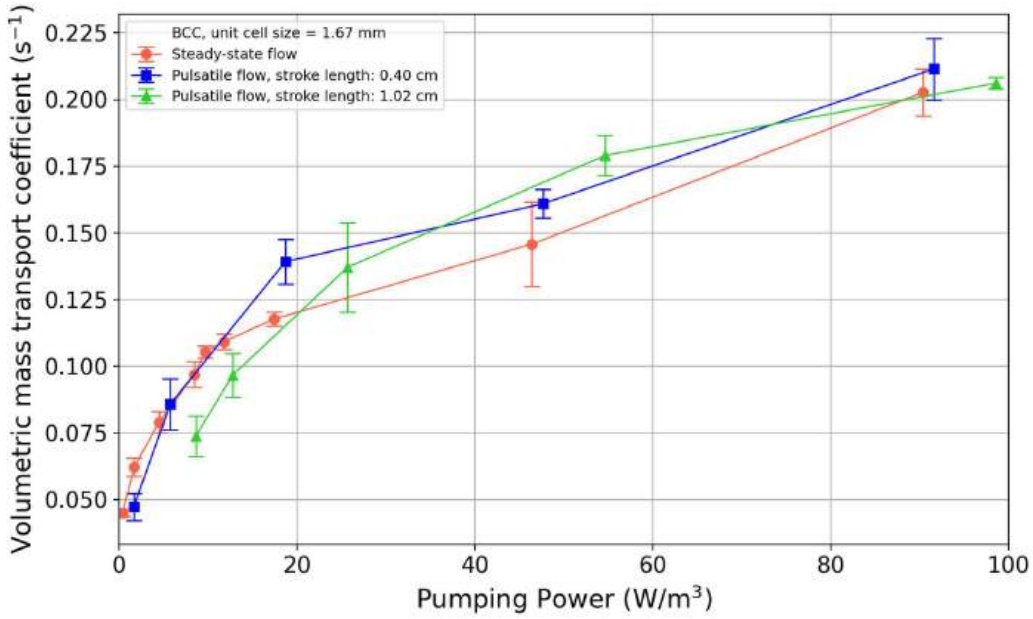

Fig. 1. Volumetric mass transport coefficient as a function of electrolyte pumping power for steady-state and pulsatile flow in a 3D-printed electrode. The electrolyte flow velocity for steady-state flow and for pulsatile flow with stroke lengths of 0.40 cm and 1.02 cm ranges from 0.35 to 5.37 cm/s. All pulsatile flow pulses at a frequency of 1 Hz. The error bar represents standard deviation of n=3 measurements.

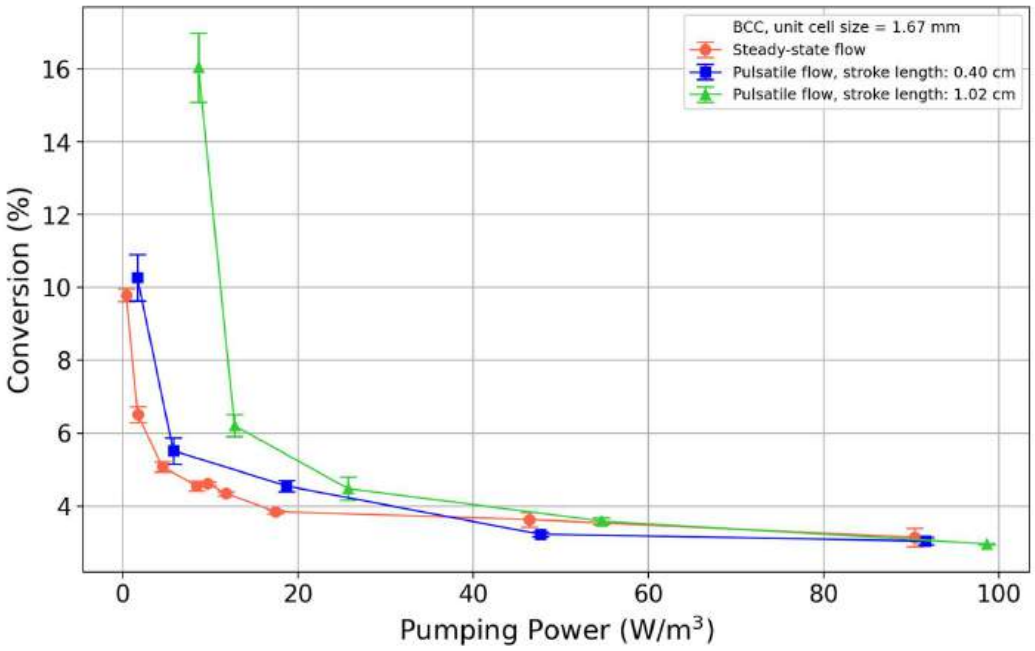

Fig. 2. Conversion as a function of electrolyte pumping power for steady-state and pulsatile flow in a 3D-printed electrode. The electrolyte flow velocity for steady-state flow and for pulsatile flow with stroke lengths of 0.40 cm and 1.02 cm ranges from 0.35 to 5.37 cm/s. All pulsatile flow pulses at a frequency of 1 Hz. The error bar represents standard deviation of n=3 measurements.

Acknowledgements: This work was funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. This work is supported by ERC grant RECHARGE (Project No. 101115100, DOI: 10.3030/101115100).

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EES - D3 - O06
High performance LSCs based on PMMA/oligothiophene thin films: A slot die coating approach

Irene Motta[1,2], Andrea Trifoglio[3], Massimo Zambianchi[3], Manuela Melucci[3], Gregorio Bottaro[2,4], Lidia Armelao[1,4,5]
[1]Dept. of Chemical Sciences (DiSC), University of Padova, IT; [2]Institute of Condensed Matter Chemistry and Technologies for Energy (ICMATE), National Research Council (CNR), c/o Dept. of Chemical Sciences (DiSC), University of Padova, IT; [3]Institute for Organic Synthesis and Photoreactivity, National Research Council (CNR), IT; [4]National Interuniversity Consortium of Materials Science and Technology (INSTM), IT; [5]Dept. of Chemical Sciences and Materials Technologies (DSCTM), National Research Council (CNR), IT

Luminescent solar concentrators (LSCs) are known in the field of building-integrated photovoltaics (BIPVs) as light management devices that can be installed in place of transparent or semi-transparent building elements. They are typically comprised of a fluorescent slate coupled to a photovoltaic component capable of harvesting the fluorescence emitted light and generating electricity. Emission is produced by a fluorophore embedded into the slate or coated onto a substrate in the form of a film.
Herein we report a series of LSCs based on poly(methyl methacrylate) (PMMA) films doped with strongly fluorescent thiophene oligomers, coated onto glass substrates using slot die coating. Thiophene oligomers possess suitable properties for LSC development, as efficient broadband absorption, high photoluminescence quantum yield and prolonged photostability. Two state-of-the-art dyes, Lumogen Red 305 and Coumarin 6, have also been included in the study as benchmark compounds.
The films have been realized through an optimized slot die coating procedure (**Fig. 1**), ensuring high optical quality and excellent reproducibility among samples, especially in terms of thickness homogeneity (30 ± 3 mm across a 50 × 50 mm^2 substrate area, **Fig. 2**). Slot die coating is also an easily scalable technique, already widely implemented at an industrial level.
The fluorophores have been fully characterized before and after embedment into the polymer, to investigate any effect of material processing on their photophysical properties. The LSC-PV devices have then been realized by edge-coupling the coated glass slates to Si PV cells. Relevant electrical characterizations, as current density-voltage curves and external quantum efficiency spectra measurements, have been conducted in compliance with well-established guidelines for LSC reporting. The oligothiophene-doped LSCs display excellent performance, with electrical outputs and photostability comparable to the benchmarks, while providing with alternative colorations and lower visual impact, both important aspects to consider for BIPV applications.

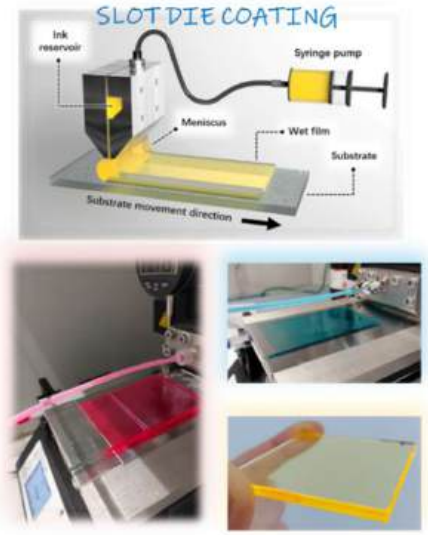

Fig. 1. Top: Schematic illustration of the slot die coating process. Bottom: Photograph of the fabricated coatings, with dimensions of 50 × 50 mm² or 50 × 80 mm².

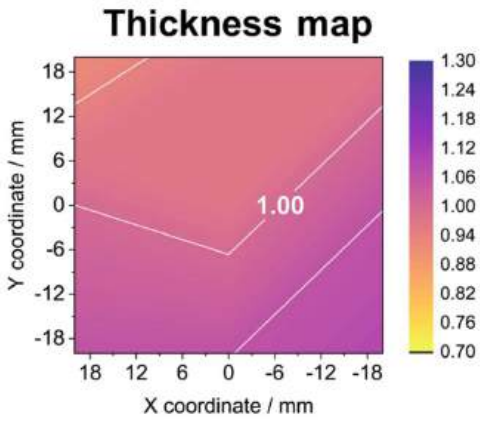

Fig. 2. Spatial photoluminescence distribution across a representative 30 µm thick LSC, illustrating the high homogeneity of the coating.

EES - D3 - O07

Non-equilibrium electrochemical synthesis of metastable Cu-In intermetallic compounds for CO_2 electroreduction

Soichi Kikkawa[1], Tatsuya Koubayashi[1], Toshiaki Oka[1], Takeshi Watanabe[2], Tetsuo Homma[2], Hideyuki Kawasoko[1], Seiji Yamazoe[1*]

[1]Graduate School of Science, Tokyo Metropolitan University, JP; [2]Japan Synchrotron Radiation Research Institute, JP

Electrochemical CO_2 reduction reaction (eCO_2RR) has attracted attention for carbon utilization driven by renewable electricity.[1,2] Tailoring catalyst surfaces to promote eCO_2RR while suppressing the competing hydrogen evolution reaction (HER) remains a key challenge. Intermetallic compounds (IMCs), which possess well-defined atomic arrangements and electronic structures, represent a platform for catalyst design.[3,4] Here, we report the non-equilibrium synthesis of IMCs via electrochemical reduction of mixed metal oxide precursors and their application to selective eCO_2RR.

The electrochemical reduction was carried out in an H-type cell at −1.5 $V_{Ag/AgCl}$, and investigated by powder X-ray diffraction (PXRD). Reduction of Cu–In mixed oxide precursor resulted in the formation of $CuIn_2$ and Cu_2In. Notably, $CuIn_2$ is a thermodynamically metastable phase inaccessible by conventional thermal synthesis,[5] highlighting the non-equilibrium nature. The resulting $CuIn_2$ located on the surface of core-shell like particle produced eCO_2RR products, namely CO and formate while suppressing HER, achieving a Faradaic efficiency of 88% for eCO_2RR (Figure 1). In contrast, a physical mixture of CuO and In_2O_3 showed poor eCO_2RR selectivity, highlighting the importance of mixed-oxide precursors. [6]

Furthermore, operando X-ray absorption spectroscopy combined with X-ray diffraction (XAS–XRD) directly revealed the dynamic reduction of mixed metal oxides and the concurrent observation of crystalline phases. X-ray absorption near-edge structure analysis showed that In species in Cu–In mixed oxide were reduced preferentially to Cu species, while XRD revealed that the emergence of IMC phases exhibited an induction period relative to the decomposition of Cu–In mixed oxide. These results demonstrate a versatile route to access thermally metastable Cu–In IMC and offer new opportunities for the rational design of catalysts for selective eCO_2RR.

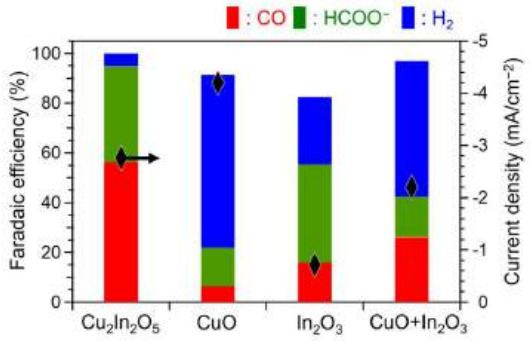

Fig. 1. Faradaic efficiency and current density in eCO_2RR.

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EES - D3 - O08

2H-MoS_2-supported nickel single-atom catalysts for the enhanced photoelectrocatalytic hydrogen production from water splitting

Hepsiba Niruba Catherine[1], Deblina Roy[1], Ruey-An-Doong[1*]
[1]Institute of Analytical and Environmental Science, National Tsing Hua University, TW

Single-atom catalysts (SACs) featuring precise coordination environments present an effective and low-cost strategy for photoelectrocatalytic (PEC) hydrogen production from water splitting. In this study, an atomically dispersed nickel SAC (Ni_{SAC}) on 2H-MoS_2 has been fabricated via an efficient hydrothermal strategy. Different Ni amounts at 1-5 wt% (Ni_{SAC}) were atomically dispersed onto 2H-phase molybdenum disulfide (Ni_{SAC}@2H-MoS_2) through a hydrothermal synthesis at 200 °C to serve as the photocathode for H_2 production evolved from water splitting. The electron microscopy image and XPS results show that Ni_{SAC}, with an average diameter of 0.17 nm, is atomically dispersed onto 2H-MoS_2. The Ni K-edge EXAFS analysis shows the absence of Ni–Ni coordination, and a dominant Ni–S coordination shell with a bond length of 2.18 Å and a coordination number of 5.78 is observed. The Ni active sites serve as electron sinks, efficiently trapping photogenerated electrons and suppressing electron–hole recombination, and an optimized 2.5 wt% Ni_{SAC}@2H-MoS_2 can achieve a H_2 production rate of 8.78 mmol g^{-1} h^{-1} with remarkable stability over 2 h upon applying −0.1 V vs. RHE. The remarkable PEC water splitting is ascribed to the synergistic effect of the intrinsic electric field in 2H-MoS_2 and the Schottky barrier at the Ni_{SAC} and 2H-MoS_2 interface, which induces downward band bending and promotes directional charge transfer toward the Ni sites to effectively produce H_2 from water splitting. Moreover, the Ni_{SAC}@2H-MoS_2 PEC nanocatalyst exhibits excellent long-term operational stability under continuous solar irradiation, further supporting its practical viability for H_2 production. Results of this study highlight the potential of developing the atomically dispersed Ni catalysts as sustainable, noble-metal-free cocatalysts for large-scale solar-to-hydrogen conversion. The solid results of this study can form an integrated platform to develop next-generation, noble-metal-free photocathodes for sustainable and cost-effective solar-to-hydrogen energy conversion.

EES - D3 - O09

Maltodextrin-based electrolytes at work in safe aqueous dye-sensitized solar cells for ambient light harvesting

Luca M. Cavinato[1], Giovanni Spinelli[1], Nadia Barbero[1], Francesco Trotta[1], Claudia Barolo[1,2,3], Marco Zanetti[1,2,3], Claudio Cecone[1], Simone Galliano[1,2]

[1]Dept. of Chemistry, Università degli Studi di Torino, IT; [2]Instm Reference Centre, IT; [3]ICxT Interdepartmental Centre, Università degli Studi di Torino, IT

As demand grows for autonomous low-power electronics—such as **IoT devices**, indoor photovoltaics are becoming a key enabling technology. Among the various IPV technologies, Dye-Sensitized Solar Cells (DSSCs) have shown significant promise due to their high efficiency under ambient lighting, low fabrication cost, and mechanical flexibility.[1] Current DSSCs electrolytes typically rely on redox mediators dissolved in **volatile and toxic organic solvents**. These pose **safety and health risks** in enclosed environments.[2] Bio-derived *quasi-solid-state* electrolytes—particularly those based on polysaccharides—offer a sustainable and safer alternative. While outdoor and indoor PCEs of 7–8% and up to 20%, respectively, have been reported using such materials with thermal stability up to 60 °C and operational lifetimes >1500 h,[3] most systems rely on *unmodified polysaccharides* and *lack a systematic study* for optimization. In this study, we present a **rational design** approach for aqueous *quasi-solid* electrolytes using maltodextrin-derived nanosponges with tailored cross-linking densities and iodine-based redox couples. The electrolytes were subjected to comprehensive electrochemical characterization, including electrochemical impedance spectroscopy (EIS), Tafel polarization, and ionic conductivity measurements. These were integrated with DSSCs device testing under outdoor and indoor illumination conditions, evaluating Voc, Jsc, fill factor, and overall power conversion efficiency (PCE). Notably, DSSCs based on the optimized *quasi*-solid electrolytes retain their PCE after >1,000 hours of shelf storage. Finally, **Multivariate Linear Analysis** was employed to correlate structural and rheological properties (*e.g.,* swelling ratio, viscosity, I_2 uptake) with key electrochemical and photovoltaic metrics, enabling the identification of dominant factors controlling performance. This data-driven approach provides quantitative design guidelines for future electrolyte development, highlighting the tunability of polysaccharide-based matrices for indoor photovoltaic-specific operating conditions.

Overall, this work advances the field by combining biopolymer engineering, electrochemical analysis, and multivariate data modeling to deliver safe, stable, and high-performing electrolytes for indoor DSSCs.

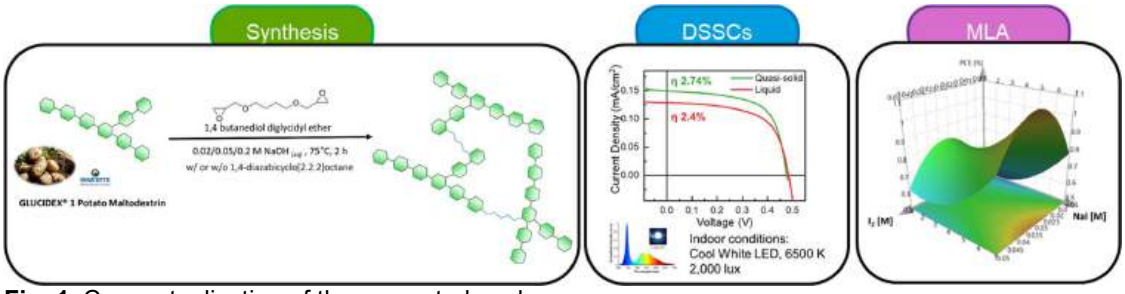

Fig. 1. Conceptualization of the presented work.

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EES - D3 - O10
Boosting the quantum efficiency of ionic carbon nitrides for solar-driven fuel synthesis

Christian Mark Pelicano[1]
[1]*Max Planck Institute of Colloids and Interfaces, DE*

Solar-driven catalysis offers a sustainable route to produce valuable fuels. Metal poly(heptazine imide) (MPHI), a crystalline ionic carbon nitride, has emerged as an efficient photocatalyst due to its favorable band alignment for H_2O_2 and O_2 evolution. Crucially, enhancing and shifting the light absorption of PHI into the visible region is essential for maximizing solar energy utilization. Here, we summarize recent advances in boosting the quantum efficiency of MPHI. We found that introducing oxamide during KPHI synthesis induces lattice distortion and activates n→π* transitions, extending solar absorption and improving H_2O_2 production; the optimized catalyst reached an AQY of 41% at 410 nm. Further gains were achieved by incorporating NH_4Cl, which fragments KPHI into distorted nanocrystals, raising the AQY to 49% at 410 nm and 5% at 525 nm—the highest for metal-free H_2O_2 photocatalysts. Additionally, $NaBH_4$ treatment enabled B doping and N defects, yielding an AQY of 4.57% at 420 nm for oxygen evolution. Future efforts will focus on precise electronic-structure engineering to further extend visible-light absorption while maintaining high charge-separation efficiency.

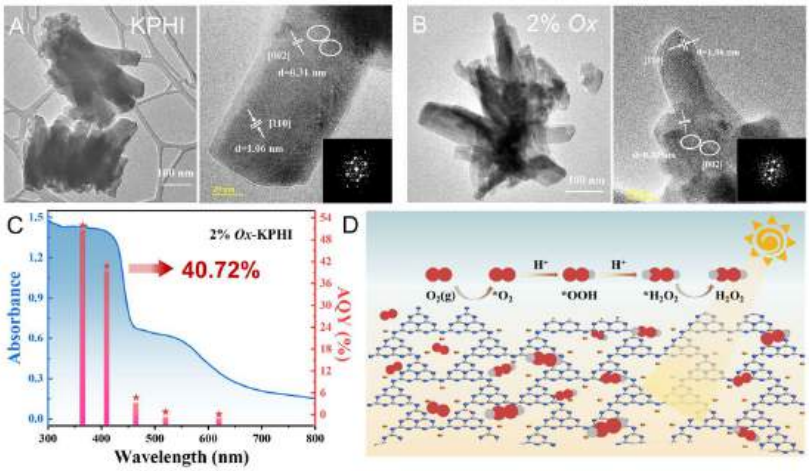

Fig. 1. (A) HRTEM images of KPHI and (B) *2%Ox*-KPHI. (C) UV-Vis spectrum and AQY values for *2%Ox*-KPHI as a function of the irradiation wavelength. (D) Schematic diagram of H_2O_2 production over *2%Ox*-KPHI through photocatalytic ORR.

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EES - D3 - O11

Substituting selenium for sulfur for efficient tuning of properties in $BaZrS_3$ perovskite for photovoltaic applications

Lorenza Romagnoli[1], Andrea Ciccioli[1], Alessandro Latini[1]
[1]*Sapienza University of Rome, IT*

Chalcogenide perovskites have been proposed as alternative to hybrid halide perovskites for photovoltaics, thanks to superior thermal and chemical stability. $BaZrS_3$, with band gap in the range 1.7 – 1.9 eV, is a potential candidate as top absorber in tandem solar cells; however, strategies to lower the gap to the ideal value of 1.34 eV for a single-junction cell, are actively sought. Among these, alloying $BaZrS_3$ with other elements has been suggested theoretically, and substitution of Ti for Zr has been experimentally performed, showing band gap reduction upon addition of 10% Ti, and phase segregation for higher amounts[1]. Substitution of Se for S has also been predicted to lower the band gap of $BaZrS_3$, nevertheless experimental reports in this sense are practically absent, so extensive work is essential to assess this as an efficient way for band gap tuning.
Herein, we describe the synthesis of solid solutions $BaZrS_{3-x}Se_x$, prepared following a recently developed methodology for $BaZrS_3$, $BaHfS_3$ and their solid solutions[2], using relatively mild conditions (16 hours at 500 °C), and their characterization through powder XRD, UV-visible and Raman spectroscopy. Results reveal that sulfur substitution with selenium with retention of perovskite structure is possible up to a certain Se concentration, with formation of phases different from the perovskite one after that concentration. Nevertheless, reduction of band gap value with increasing Se content, along with expansion of the unit cell, are observed, validating theoretical predictions. This study confirms Se-alloying as a practical way to tune structural and opto-electronic properties of chalcogenide perovskites and extends the scope of our new synthetic method.

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EES - D3 - O12

Precursor-driven reconfiguration of bulk and interface enhances the solar-driven water splitting performance of carbon nitride photoanode

Abraham Kasa[1,2,3], Lakshman Sundar Arumugam[4], Anja Vanleenhove[5], Vishal Jose[1,2,3], Thierry Conard[5], Daniely Santos[1,2,3], Jan D'Haen[1], Angelica Simbula[6], Laurence Lutsen[1], Javier E. Durantini[4], Sixto Giménez[4], Guy Brammertz[1,2,3], Sudhanshu Shukla[1,2,3], Bart Vermang[1,2,3]

[1]Hasselt University, BE; [2]EnergyVille, BE; [3]imec, Imo-imomec, BE; [4]Institute of Advanced Materials (INAM), Universitat Jaume I, ES; [5]imec, BE; [6]Università di Cagliari, IT

Photoelectrochemical (PEC) solar energy conversion is a promising technology to address the growing global energy demand, which is projected to exceed 30 TW by 2050[1]. This approach enables the replacement of polluting energy sources with clean and sustainable energy harvested directly from sunlight[2]. Carbon nitride (CN) has emerged as a promising metal-free semiconductor for PEC watersplitting applications[3]. However, its practical implementation is hindered by low photoactivity compared to inorganic photoanodes. Here, we report the excellent photoactivity of modified CN photoanodes for PEC water-oxidation. Incorporating powder precursors during thermal polymerization led to favorable morphological modifications, improved structural ordering, and reduced charge transfer resistance. The powder thiourea-assisted growth of CN boosted the photocurrent by almost 3-fold. This enhancement is attributed to suppressed carrier recombination, improved charge transfer, and the formation of CN and SnS2 heterojunctions. The champion CN photoanode achieved an excellent charge extraction efficiency of up to 69% and a benchmark photocurrent density with and without a hole scavenger of about 2.7 and 2 mA cm^{-2}, respectively for water oxidation at 1.23 V versus RHE in neutral 0.1 M Na_2SO_4 solution, with an onset potential of 0.32 V vs RHE and external quantum yield reaching 42% at 440 nm. This strategy demonstrates excellent PEC performance, advancing the potential of this material for practical applications in PEC systems

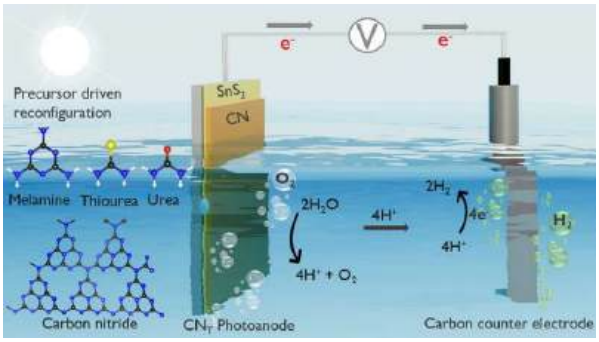

Fig. 1. PEC water oxidation by CN photoanodes

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EES - D3 - O13

An operando AP-NEXAFS study on CO_2 photoreduction with Cu-NPs supported by photoactive materials

Giulia Forghieri[1], Silvia Mauri[2], Elena Ghedini[3], Piero Torelli[2], Michela Signoretto[1]
[1]Ca' Foscari University and INSTM RU of Venice Dept. of Molecular Sciences and Nanosystems IT; [2]CNR-Istituto Officina dei Materiali TASC, IT; [3]University of Bari Aldo Moro Dept. of Chemistry, IT

Using light and water vapor to reduce CO_2 into various carbon-based products, such as methane, is a promising strategy to achieve CO_2 conversion into useful products[1]. Copper (Cu) is a well-studied photocatalyst due to its high affinity for carbon intermediates, favouring CO_2 evolution (CER) over hydrogen evolution reaction (HER). In fact, various studies revealed that CuO can act both as catalyst and as reactant during the photocatalytic process[2,3]. Recently we have shown that adding CuO nanoparticles to light sensitive materials like $BaTiO_3$ (BTO) and TiO_2 enhance the photocatalytic performance of the material[4]. Therefore, to elucidate the interaction between CuO nanoparticles and support materials, near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy was utilized as tool for investigating the electronic structure and redox behavior of the catalysts[5]. This study was carried out at ambient pressure to explore the redox behavior of CuO-NPs in CuO-BTO and CuO-TiO_2 photocatalysts in operando CO_2 photoreaction conditions. The experiment confirmed the enhanced methanation on the CuO-BTO system over TiO_2 based catalyst. Moreover, thanks to the NEXAFS analysis we were able to establish that the activity of both catalyst is linked to the formation of a reversible redox couple Cu^+/Cu^{2+} and that in the CuO-BTO sample the light illumination causes a charge transfer between support and the CuO nano-particles thus enhancing the redox activity. Finally, based on the evidence collected, we were able to propose an alternative reaction pathway for CO_2 conversion by BTO materials (Figure 1).

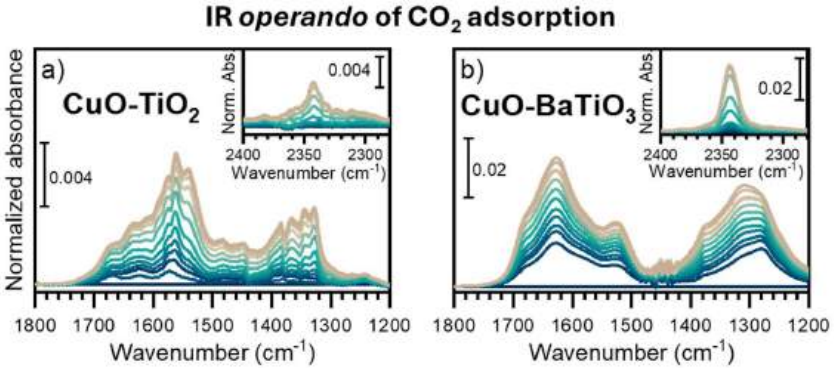

Fig. 2. Different interaction of CuO-TiO_2 and CuO/BTO with CO_2.

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EES - D3 - O14

A green chemistry strategy for rare earth element recovery from acid mine drainage using living biomass

Thainara Viana[1*], Nicole Ferreira[1,2], Eduarda Pereira[1], Bruno Henriques[1]
[1]*LAQV-REQUIMTE – Associated Laboratory for Green Chemistry, Dept. of Chemistry, University of Aveiro, PT;*
[2]*CICECO, Department of Chemistry, University of Aveiro, PT*

The transition to clean technologies is critically dependent on rare-earth-elements (REE); however, their conventional extraction is associated with significant environmental impacts, including acidic effluents, particulate matter, and radioactive residues[1]. Consequently, sustainable alternative REE sources are increasingly being explored, particularly secondary resources such as waste electrical and electronic equipment, industrial by-products, and acid mine drainage (AMD). Among these, AMD is especially attractive because REE are already dissolved in aqueous matrices compatible with established chemical separation and recovery processes. Recovering REE from AMD enables resource valorisation while mitigating mining-related environmental impacts, supporting circular economy principles[2]. Biosorption using low-cost, renewable materials has emerged as a promising strategy for metal recovery. Seaweeds are particularly attractive due to their chemical composition, rich in functional groups capable of binding metal ions, and their minimal processing requirements[3]. However, most previous studies rely on synthetic solutions, and the feasibility of REE recovery using living biomass in real AMD remains insufficiently explored.

In this study, living seaweed (*Gracilaria* sp.) was evaluated for REE removal, concentration, and recovery from raw AMD. Optimised biosorption conditions were applied[4], followed by thermal treatment of the biomass to pre-concentrate sorbed REE. Calcination and microwave-assisted pyrolysis increased ΣREE concentrations by 7–10 times while reducing biomass mass by 87.7–92.0% at 600–900 °C. Lower-energy conditions were also assessed. Thermal treatment at 400 °C resulted in lower REE enrichment, whereas at 600 °C with reduced residence time enhanced ΣREE concentration while maintaining high mass loss (~91%).

Overall, integrating biosorption with optimised thermal processing provides a green, low-impact, and resource-efficient strategy for REE recovery from real AMD waters.

This work is funded by COMPETE2030-FEDER-00847800 and national funds from FCT/MCTES through project UID/50006— Laboratório Associado para a Química Verde—Tecnologias e Processos Limpos. Thainara Viana and Nicole Ferreira thank FCT/MCTES for PhD grant ref. 2022.13015.BD and 2022.13017.BD, respectively.

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EES - D3 - O15

Integrated subcritical water extraction and membrane/resin fractionation for circular valorisation: Chestnut wood residues into tannin-based biopolymers

Giorgio Grillo[1], Clelia Aimone[1], Giorgio Capaldi[1], E. Calcio Gaudino[1], Anastasia Anceschi[2], Alessia Patrucco[2], Silvia Bonetta[3], Giancarlo Cravotto[1]

[1]Dept. of Drug Science and Technology, University of Turin, IT; [2]Institute of Intelligent Industrial Technologies and Systems for Advanced, Manufacturing (STIIMA), IT; [3]Dept. of Life Sciences and Systems Biology, University of Turin, IT

Aligned with circular-economy and green-extraction principles, this work presents an integrated route to valorise chestnut wood (*Castanea sativa* Mill.) residues, a polyphenol-rich lignocellulosic matrix, into high-value fractions and functional bio-based materials. [1] A water-only, process-intensified extraction was developed through Microwave-Assisted Subcritical Water Extraction (MASWE) and optimized by Central Composite Design (176 °C, 14 min, S/L 1:20) to maximize recovery while modulating the balance between low-molecular-weight phenolics and tannins. The resulting crude extract was upgraded via a molecular-weight cascade filtration (ultrafiltration followed by nanofiltration) coupled with resin adsorption/desorption (also CCD-optimized), enabling selective enrichment, efficient purification, and extensive water recirculation, achieving 89.2% overall recovery. [2]

All streams were characterized for total phenolics, antioxidant capacity, tannins, and sugars, and evaluated for bioactivity (enzyme inhibition and antimicrobial performance). The most active fraction, highly enriched in tannins (≈80%), was incorporated into an innovative PVA-based formulation and further reinforced with a pectin-rich orange peel co-extract, improving mechanical performance while increasing renewable-carbon content. The resulting composite showed promising physicochemical behaviour and antioxidant properties, together with notable biodegradability. In parallel, the recovered fractions displayed inhibitory activity against multiple bacterial targets, including *Pseudomonas aeruginosa*, *Salmonella Typhimurium*, and *Escherichia coli*, supporting their potential as functional additives.

Overall, the proposed MASWE–membrane/resin platform enables a scalable, water-based biorefinery strategy that couples solvent minimization, process intensification, and separation-driven selectivity to convert underutilized biomass residues into multiple value streams and biodegradable materials.

Fig. 1. Chestnut Wood Waste valorisation scheme.

Acknowledgment: Grant for Internationalization – GFI (2021-2023), Project: TANNFRACT.

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EES - D3 - O16

From Industrial Waste to Smart Windows: Circular Recovery and Upcycling of Vanadium for Advanced Thermochromic Coatings

Lisa Royer[1,2], Kimberly Timmers[1,2], Jordi Volders[1,2], Cindy P. K. Yeung[1,2], Daniel Mann[1,2,3] Pascal Buskens[1,2,3]*
[1]The Netherlands Organisation for Applied Scientific Research (TNO), NL; [2] Brightlands Materials Center, NL; [3]Institute for Materials Research (imo-imomec), DESINe Group, Hasselt University, BE

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Vanadium is used in steel production, energy storage, and catalysis, yet its disposal poses significant environmental and economic challenges. This study presents a circular approach for the recovery and upcycling of vanadium from an industrial waste catalyst, transforming it into vanadium pentoxide (V_2O_5): a suitable precursor for advanced VO_2-based thermochromic coatings. These coatings autonomously switch between an infra-red (IR) light blocking and an IR transparent state at a specific transition temperature, while staying visibly transparent thanks to the reversible transition of VO_2 from a monoclinic (M) to a rutile (R) crystalline structure. This type of coating finds its application in smart windows, decreasing the energy use of a typical Dutch household of up to 24% [1,2,3]

The spent catalyst is composed of aluminium, iron and vanadium compounds. Using a combination of reductive acid leaching, oxidation, and selective precipitation steps, pure V_2O_5 (99.97% purity - Figure 1A) was extracted from the spent catalyst with an 82% yield. This overcomes the purity and yield obtained in the literature[4,5]. This material was subsequently converted, into monoclinic VO_2(M) as part of a thermochromic coating on a glass substrate. Optical measurements (Figure 1B) revealed a visible transmittance of 55% and a solar modulation of 4.4%, correlating well with literature values[3]. This process demonstrates the feasibility of upcycling industrial vanadium waste into functional materials for smart windows, contributing to resource efficiency and environmental sustainability.

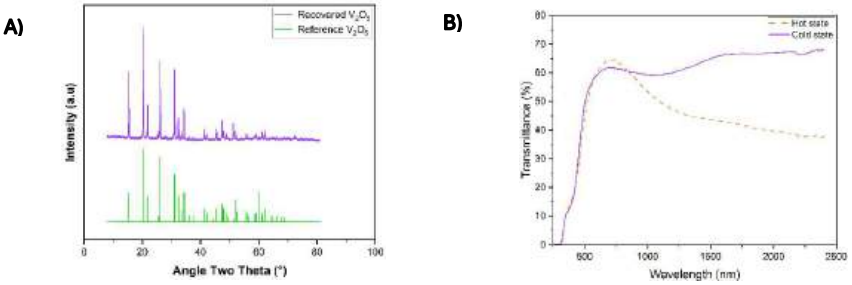

Figure 2: A) Diffractogram of the recycled V_2O_5 (purple) compared to PDF card 00-009-0387 (green). B) Transmittance curves below and above the transition temperature of the VO_2 coating made from recycled material.

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ESS - D3 - O17
Impact of mixed polymer streams and contaminants on radical-initiated polymer degradation

Roy B. Maas[1], Sophie H. van Vreeswijk[1], Eelco T.C. Vogt[1], Florian Meirer[1], Bert M. Weckhuysen[1]
[1]Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry, Dept. of Chemistry, Utrecht University, NL

To achieve circularity for polyolefins, chemical recycling strategies must operate at low temperatures and exhibit high activity and selectivity toward valuable products.[1] While the use of solid acid catalysts presents an effective strategy for this[2,3], depolymerization of polypropylene (PP) is strongly limited by mass-transfer constraints, as high-molecular weight melts cannot effectively access catalytic active sites.[4] In this work, we investigate peroxide pretreatment using 2,5-dimethyl-2,5-di-(tert-butylperoxy)hexane (DBPH) to induce β-scission and reduce the molecular weight (M_w) of PP prior to catalytic conversion. Isotactic PP (M_w = 55,000 g mol^{-1}) was treated with 0-10 wt.% DBPH at 180 °C under Ar (1 bar) without stirring. Thermogravimetric analysis (TGA) reveals that 5 wt.% DBPH lowers the cracking temperature of PP by ~80 °C, indicating potential energy savings. Gel permeation chromatography (GPC) shows a concurrent minimum in Mw at 5 wt.% DBPH, confirming that peroxide-assisted chain fragmentation is responsible for the improved cracking behavior. Furthermore, Fourier transform infrared (FTIR) spectroscopy shows an increase in vinylidene content with peroxide loading. Finally, nuclear magnetic resonance (NMR) reveals vinylidene signals in terminal and internal isomers, with the latter arising from disproportionation driven by high local radical concentrations. In conclusion, at 5 wt.% DBPH, β-scission dominates yielding the greatest M_w reduction, improving polymer-catalyst interactions and lowering the energy required for subsequent depolymerization. In real waste streams, however, post-consumer plastic waste is composed of mixed polymer streams (e.g., PP, PE, PS, PET, and PVC)[5] and contain impurities, such as inorganic ions[6] (e.g., Cu^{2+}, Mg^{2+}, and Ca^{2+}) and organic additives, like plasticizers, that can influence radical formation, propagation, and termination during peroxide-assisted degradation. Therefore, the impact of these constituents on peroxide-assisted degradation is systematically evaluated and compared with pristine PP to assess practical applicability. This study demonstrates the potential of peroxide-assisted pretreatment for recycling plastic representative of real waste streams.

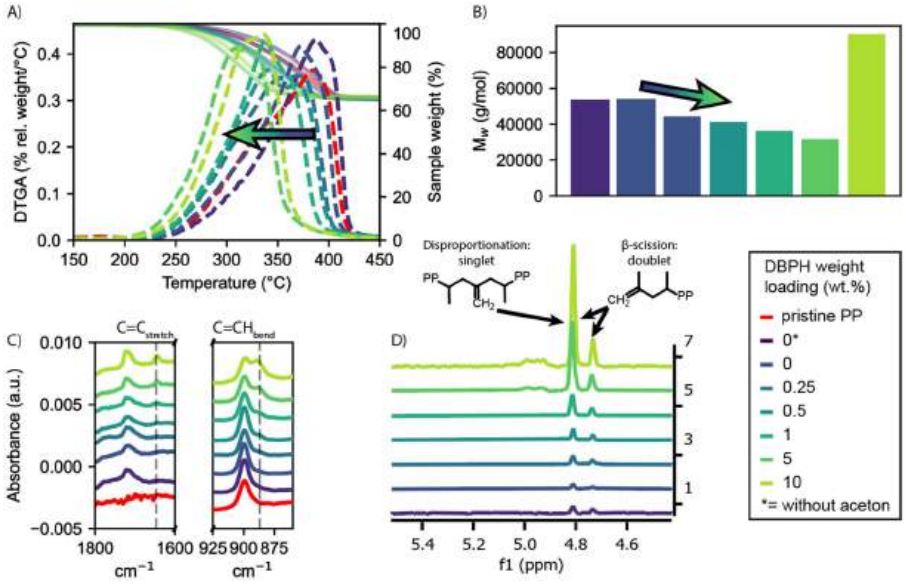

Fig. 1. (A) Thermogravimetric (TGA) profiles showing weight loss of PP on a bed of FCC-Ecat catalyst (PP: catalyst ratio =1:2 by weight). Relative sample weight (%) is shown on the right-axis and the derivative of the weight loss on the left-axis as a function of temperature (°C). (B) Gel permeation chromatography (GPC) analysis showing a decrease in M_w with increasing DBPH concentration up to 10wt.%. (C) Infrared (IR) stacked spectra highlighting the formation of vinylidene functional groups at ~ 1647 and ~ 889 cm^{-1} (dashed lines). (D) Nuclear magnetic resonance (NMR) stacked spectra showing overlapping singlet of internal vinylidene at ~ 4.81 ppm and a doublet of terminal vinylidene at ~ 4.81 and ~ 4.72 ppm.

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EES - D3 - O18
Statistical entropy analysis for the evaluation of polymer complexity and circularity

Attila Kovacs[1], Cristina Moyaert[1], Yoshi W. Marien[1,2], Carla Carelo Pérez[3], Paul H.M. Van Steenberge[2], Dagmar R. D'hooge[2,4], Philippe Nimmegeers[5,6,7], Pieter Billen[1]
[1]iPRACS research group, Faculty of Applied Engineering, University of Antwerp, BE; [2]Laboratory for Chemical Technology, Ghent University, BE; [3]School of Industrial Engineering, Technical University of Valencia, ES; [4]Centre for Textile Science and Engineering, Ghent University, BE; [5]Dept. of Engineering Management, Faculty of Business and Economics, University of Antwerp, BE; [6]Flanders Make@UAntwerp, BE; [7] NANOlight Centre of Excellence, University of Antwerp, BE

Improving the performance and circularity of polymer systems requires making trade-offs. Improving the mechanical or chemical properties of polymers often involves increasing structural diversity (e.g., copolymerization, grafting, and cross-linking). However, this simultaneously raises the barrier associated with the complexity and energy demand of separation and efficient material recovery during recycling. Unfortunately, current polymer descriptors (e.g., net composition, dispersity, or average molar mass) that describe the evolution of polymer systems during virgin production are inadequate for guiding circular design strategies.
To overcome these limitations, we propose using statistical entropy analysis (SEA) to describe the global complexity of polymer systems. Based on Shannon's information theory, SEA can describe the complexity of material distributions in systems[1,2]. Using SEA, we introduce a multilevel phenomenological model that captures the emerging structural diversity during polymer synthesis at the following hierarchical levels: (1) chain length, (2) occurrence of grafts, (3) graft length, and (4) monomer identity.
In this study, we examined whether the proposed multilevel molecular SEA can capture the following: (A) increasing structural complexity as a function of monomer conversion, (B) increasing complexity when blending polymers of different qualities, and (C) exceeding the performance of conventional descriptors in tracking complexity. As a case study, we examined the free radical-induced grafting (FRIG) of polybutadiene with styrene as a function of monomer conversion. We used kinetic Monte Carlo simulations to generate realistic molecular distributions. Calculations based on number- and mass-fraction distributions revealed that the latter is more sensitive to changes in polymer complexity. Entropy also exhibited a stronger correlation with polymer complexity as a function of conversion than dispersity did. Mixing different-quality polymer feedstocks increased entropy. These results demonstrate the potential of the proposed multilevel entropy approach for quantifying polymer complexity and supporting polymer development that balances performance requirements and circularity objectives from the earliest design stages.

This research is part of the RESTEP FWO junior fundamental research project (grant number G027122N).

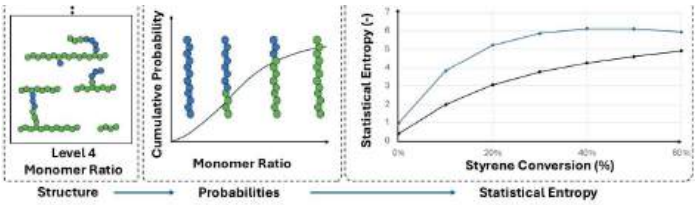

Fig. 3: The evolution of entropy as a function of monomer conversion is calculated using the mass-fraction probability distribution based on the kinetic Monte Carlo simulation of the polymer structure.

Philippe Nimmegeers and Yoshi W. Marien hold FWO senior postdoctoral fellowship (grant number: 1215523N/12B3Y24N).

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EES - D3 - O19
Hydrothermal pretreatment improving in-situ catalytic pyrolysis of plastic waste feedstocks

Hendrik Van Leuven[1], Brent Smeyers[1], Kseniia Vikanova[1], Bert Lagrain[1], Bert F. Sels[1]
[1]KU Leuven, BE

7The rising volume of postconsumer plastic waste (PCW) necessitates recycling strategies capable of processing highly contaminated post-consumer feedstocks (figure 1). direct feedstock-catalyst contact, or in-situ catalytic pyrolysis is a promising chemical recycling route to selectively convert PCW into valuable chemicals such as light olefins, naphtha or BTX fractions.[1] However, catalyst deactivation caused by feedstock impurities (i.e., polymer sorting errors, (in)organic additives and use phase contaminants) remains a key challenge that needs to be addressed.
From an in-house developed two-dimensional thermogravimetric analysis (2D-TGA) method, two promising catalysts are taken as model catalysts: a zeolite catalyst and an amorphous silica alumina catalyst.[2] Upon reaction with PCW feedstocks, both catalysts show high degrees of deactivation.
In this work, a hydrothermal pretreatment strategy for sorted PCW waste mitigates deactivation from multilayer polymer contaminants including polyamides (PA) and polyethylene terephthalate (PET) as well as food residues and selected additives.
Pretreatment using biphasic water/n-butanol mixtures, rather than water alone, significantly reduces the presence of catalyst-poisoning species due to hydrolysis/alcoholysis pathways. Removal of these impurities prior to catalytic conversion preserves acid catalyst activity and enhances process robustness. This impurity-focused pretreatment enables the direct catalytic valorisation of low-value post-consumer polyolefins and represents an important step toward scalable, resilient plastic recycling.

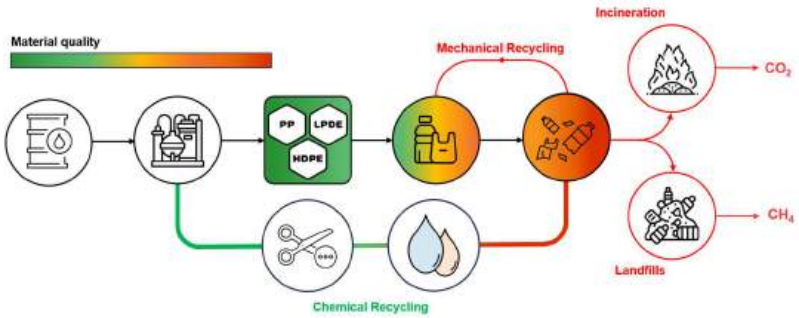

Fig. 4. schematic representation of the linear plastic economy with different end of life management options.

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EES - D3 - O20

Cross-regional LC-HRMS suspect and non-target screening of contaminants in rivers and aquaculture waters

Manuel A. Andino-Enriquez[1], Debora Fabbri[1], Federico Cristaudo[1], Federica al Bello[2], Claudio Medana[2], Paola Calza[1]

[1]Dept. of Chemistry, University of Turin, IT; [2]Dept. of Molecular Biotechnology and Health Science, University of Turin, IT

The occurrence of contaminants of emerging concern (CECs) in aquatic environments varies with geographical location and water use, reflecting anthropogenic and environmental conditions. Conventional target analysis provides quantitative information for selected compounds but captures only a limited fraction of overall chemical diversity, especially in complex matrices[1]. The integration of suspect and non-target screening using high-resolution mass spectrometry (HRMS) is essential to broaden CEC characterization. However, comparative studies across regions and water types based on harmonized analytical workflows remain scarce. In this study, river and aquaculture water samples collected in Italy and Thailand were investigated to compare CECs occurrence using a combined suspect and non-target LC-HRMS approach. Samples were characterized for key physico-chemical parameters and extracted in parallel using Oasis HLB and Envi-Carb cartridges to maximize polarity coverage prior to analysis on an Orbitrap Fusion Tribrid mass spectrometer. Data acquisition combined full-scan/ddMS² with suspect-driven inclusion lists in positive and negative ionization modes, and data processing was performed using MZmine and GNPS. The integrated workflow revealed a broad and chemically diverse range of CECs, expanding the number and diversity of detected compounds compared to target-only approaches. Identified suspects included pharmaceuticals, lifestyle-related compounds, and industrial chemicals detected across multiple sites and water matrices. Both shared and site-specific contaminants were identified between Italian and Thai samples, indicating common anthropogenic sources and localized contamination patterns. Aquaculture waters showed overlaps with river waters but also additional suspected contaminants, reflecting the influence of aquaculture practices. These findings highlight the value of harmonized suspect and non-target LC-HRMS screening for cross-regional comparison of CEC occurrence.

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EES - D3 - O21

Improved hydrophobicity of ZIF-90 metal-organic frameworks for the removal of fluorinated pollutants from water

Michele Forza[1], Eja E. Petersen[2], Romy L. Ettlinger[2], Valentina Colombo[1]
[1]Università degli studi di Milano, IT; [2]Technische Universität München, DE

Per- and polyfluoroalkyl substances (PFAS) have been widely used in industrial applications due to their high hydrophobicity, and exceptional thermal and chemical resistance. [1] However, these same properties result in their non-biodegradable nature and, consequently, in their accumulation and persistency in the environment with growing concerns on their toxicity to humans and the ecosystem. [2] All these factors explain the current efforts in the study and development of techniques to remove these “forever chemicals” from the environment. In this context, we are focusing on the synthesis and characterization of new Zeolitic Imidazolate Frameworks (ZIFs), as regenerable platforms for PFAS removal from water through adsorption processes. ZIFs features high thermal and chemical stabilities, and within them, ZIF-90 is additionally characterized by bearing an aldehyde group on the imidazole linker, thus opening the way to increasing its chemical tunability trough post-synthetic modification of the porous network via imine condensation. [3]
In this contribution I will discuss on the preparation of ZIF-90 with a greener and scalable synthesis, proving that this MOF can be easily and quantitatively obtained in a water-based synthesis at RT and ambient pressure, compared to the solvothermal DMF-based ones reported in the literature. [3] Hydrophobicity and flurophilicity of ZIF-90 has been enhanced through post-synthetic modification with fluorinated hydrazides, to obtain novel adsorbents for PFAS removal from contaminated water. These results will be also thoroughly discussed, together with the adsorption and removal properties of the obtained derivatized materials.

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EES - D3 - O22

Simultaneous determination of thirteen antidiabetic drugs in wastewater using a novel LC-MS/MS method

Amila Hajdarević[1], Silvia Lacorte[2], Jasmina Đeđibegović[1], Eirini Andreasidou[3,4], David Heath[3,4], Ester Heath[3,4], Ana Kovačič[3,4]

[1]University of Sarajevo, Faculty of Pharmacy, BA; [2]Institute of Environmental Assessment and Water Research (IDAEA-CSIC), ES; [3]Jožef Stefan Institute, Slovenia; [4]International Postgraduate School Jožef Stefan, SI

Antidiabetic drugs are consumed in large quantities for the long-term management of type II diabetes. Recently, consumption has been amplified by the increasing misuse for cosmetic weight loss in non-diabetic populations. These evolving, often unregulated, usage trends make accurately assessing population-level consumption with traditional epidemiological methods challenging. Wastewater-based epidemiology (WBE) provides a valuable tool for assessing population-level drug use by directly measuring excreted compounds in wastewater. However, antidiabetic drugs have only been sporadically detected in wastewater. Except for metformin, environmental concentration data for most antidiabetic drugs are largely lacking, particularly for newer GLP-1 receptor agonists (semaglutide) and dual GLP-1/GIP agonists (tirzepatide) whose peptide-based structure and high molecular weight pose significant analytical challenges for quantification in complex environmental matrices.To address these gaps, we developed and validated a single LC-MS/MS analytical method capable of simultaneously quantifying thirteen widely used antidiabetic drugs including: metformin, DPP-4 inhibitors (vildagliptin, linagliptin, sitagliptin), SGLT2 inhibitors (empagliflozin, dapagliflozin), sulfonylureas (gliclazide, glipizide, glibenclamide, glimepiride), repaglinide, semaglutide, and tirzepatide. The method was applied to influent and effluent samples collected from four wastewater treatment plants in Slovenia to evaluate their occurrence, removal during treatment, and suitability for WBE applications. Nine of the thirteen target compounds were detected in influent samples at concentrations above the limits of quantification. Metformin was the most abundant compound in all influent samples, followed by dapagliflozin and empagliflozin. Semaglutide was determined in all influent samples, whereas tirzepatide was not detected. Seven antidiabetic drugs were detected in the effluent, indicating incomplete removal during conventional wastewater treatment. Removal efficiencies showed high removal for metformin, SGLT2 inhibitors, and semaglutide (≈ 90–100%), whereas DPP-4 inhibitors and sulfonylureas exhibited substantially lower removal (≈ 8–30%). This study presents the first targeted analytical approach enabling the determination of antidiabetic drugs in wastewater encompassing emerging peptide-based pharmaceuticals.

EES - D3 - O23

Integrated analytical strategies supporting risk assessment of emerging contaminants in marine ecosystems

Alessandro Bollella[1,2], Guglielmo Pacchione[1,3], Federica Nigro Di Gregorio[1]

[1]National Centre for Water Safety (CeNSiA), Italian National Institute of Health, IT; [2]University of Rome "Sapienza", Dept. of Environmental Biology, IT; [3]University of Rome "Sapienza", Dept. of Chemical Science, IT

Emerging chemical contaminants pose a challenge for environmental protection and human health, particularly in marine ecosystems where dilution coexists with long-term accumulation. Among these, per- and polyfluoroalkyl substances (PFASs) are of primary concern due to their extreme persistence, high water solubility, and resistance to degradation, promoting widespread occurrence and long-range transport.

This study aimed to develop and validate a sensitive multi-residue analytical strategy for PFAS determination in seawater, designed to integrate chemical data with ecological evaluation approaches. A solid-phase extraction–liquid chromatography–tandem mass spectrometry (SPE–UPLC–MS/MS) method was optimised for the simultaneous quantification of 30 PFASs. Water samples (500 mL) were subjected to freezing and thawing prior to extraction with Oasis WAX cartridges, followed by HPLC–MS/MS analysis. Chromatographic separation employed a dual-column setup (Accucore C18 delay column and Polar Advantage II analytical column) using a methanol–water gradient containing ammonium acetate and acetic acid, ensuring retention of both short- and long-chain PFASs while minimising background contamination.

The method demonstrated excellent analytical reproducibility, chromatographic performance, and sensitivity, with detection limits of 0.01–2.5 ng/L. A matrix-adapted limit of quantification was applied to account for background contamination in blank seawater, ensuring reliable quantification of environmental samples. The analytical performance achieved enables the generation of occurrence data suitable for integration with exposure assessment models.

Application of the validated method to Mediterranean seawater samples revealed a widespread but spatially heterogeneous distribution of PFASs. Concentrations were generally below 10 ng/L, with localised maxima up to 18 ng/L in industrialised and port-influenced areas of the Eastern Adriatic and Tyrrhenian Sea, while lower levels (≤1.7 ng/L) were observed in the Western and Southern Mediterranean. The simultaneous detection of regulated PFASs and emerging substitutes confirms the suitability of the proposed strategy for supporting PFAS risk assessment in marine ecosystems.

EES - D3 - O24

Application and integration of modern trace analytical methods for remediation and pollution emission control in sewage and drinking water treatment

Roland Kallenborn[1], Jan L. Lyche[2], Katrin Vorkamp[3], Nazli Pelin Kocatürk Schumacher[4], Melesse Eshetu Moges[4], Harsha Radnaweera[4], Juliette Lepley[1,5]

*[1]Faculty of Chemistry, Biotechnology and Food Sciences (KBM), Norwegian University of Life Sciences (NMBU), NO; [2]Veterinary College, Norwegian University of Life Sciences (NMBU), NO; [3]*Dept. of Environmental Science, Aarhus U*niversity, DK; [4]Faculty of Science and Technology (RealTek), Norwegian University of Life Sciences (NMBU), NO; [5]Agroscope, Zürich, CH*

The growing complexity of contaminants and their release profiles in aquatic environments requires advanced analytical approaches to ensure effective monitoring, control, and remediation of pollution in wastewater and drinking water systems, especially in light of recent EU and international legislation. Modern trace analytical methods—such as gas and liquid chromatography coupled with tandem mass spectrometry (GC-MS/MS, LC-MS/MS)—along with emerging sensor-based technologies like optical sensors, have transformed pollutant detection at ultra-trace levels. These tools enable comprehensive monitoring of diverse contaminants, including heavy metals, pharmaceuticals, persistent organic pollutants (POPs), plastics, and plastic additives, which pose significant risks to human health and ecosystems when released in large quantities. This overview highlights the integration of state-of-the-art analytical tools within water treatment processes, focusing on their role in identifying contamination sources, optimizing remediation strategies, and ensuring regulatory compliance. Coupling advanced platforms with data-driven approaches—such as chemometrics and machine learning—enhances predictive capabilities and process control. Real-time monitoring combined with conventional treatment technologies allows utilities to optimize processes, reduce costs, and minimize environmental impacts. Case studies demonstrate improved pollutant removal efficiency and early detection of contaminants in municipal and industrial wastewater treatment plants. These findings underscore the need for interdisciplinary collaboration among analytical chemists, environmental engineers, and data scientists to develop robust frameworks for sustainable water management. The integration of modern trace analytical methods represents a critical step toward safeguarding water quality and public health for the future.

EES - D3 - O25
Exploring the use of ceramic passive samplers for urban wastewater monitoring

Damjan Rajakovic[1,2], Ida Kraševec[3], HelenProsen[3], David Heath[1], Ester Heath[1,2], Silvia Lacorte[1,4]
[1]Jožef Stefan Institute, SI; [2]International Postgraduate School Jožef Stefan, SI; [3]University of Ljubljana, Faculty of Chemistry and Chemical Technology, SI; [4]Institute of Environmental Assessment and Water Research of the Spanish Research Council (IDAEA-CSIC), ES

In 2024, the European Urban Wastewater Treatment Directive (UWWD 2024/3019) prioritises 13 micropollutants and mandates a minimum 80% removal efficiency for at least six of these compounds during treatment. This study aims to assess the use of a novel ceramic passive sampler (CPS) to measure concentrations of micropollutants in wastewater treatment plant (WWTP) influent and effluent and to estimate their removal efficiency. The CPS containing 300 mg HLB:PoraPack (2:1) sorbent was calibrated using spiked bottled water, yielding sampling rates of 0.02-15.7 mL/day and calibration constants of 0.05-56 ng/day. Concurrently, stability assessment identified hydrochlorothiazide, irbesartan, and diclofenac as the least stable (half-lives: 0.59, 1.32, and 2.90 days, respectively). The CPS were deployed at four WWTPs (influent and effluent) over 10 days, alongside 24-hour composite samples, which were extracted with SPE (200 mg Oasis HLB). All samples were analysed using LC-MS/MS. The results were compared using the Mean Percent Difference (MPD). Good comparability (48-88% on average) was achieved between the two methods. For polar compounds ($\log K_{ow} < 2$), deviations between composite and CPS measured concentrations were generally lower in effluent than in influent, owing to reduced matrix complexity. In contrast, for non-polar micropollutants, CPS recorded higher concentrations than composite samples. In both cases, benzotriazoles were detected at the highest concentrations in wastewater (296-8,000 ng/L), whereas diclofenac and hydrochlorothiazide were below the limit of detection (LOD; 257 and 1,220 ng/L, respectively). Average removal efficiencies of the 13 studied micropollutants ranged from 6% to 76% when determined using composite sampling and from 1-99% when determined using CPS, while the average removal efficiency of each WWTP was 6-56% measured using composite sampling and 1-63% using CPS. Overall, CPS is a promising tool for monitoring representative micropollutants, although further sorbent optimisation is required to improve method comparability.

EES - D3 - F01

Amorphous coordination polymers for versatile Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, and Zn^{2+} cation storage

Robert Markowski[1], Alexandru Vlad[1]
[1]*Institute of Molecular Chemistry, Materials and Catalysis, Université Catholique de Louvain, BE*

Divalent metal-ion batteries (DMBs) are emerging as compelling alternatives to lithium-ion technology, with potential advantages in volumetric energy density, cost, sustainability, and safety. Magnesium and calcium systems are particularly attractive, yet their development is constrained by strong interactions between divalent cations and rigid inorganic host structures, which limit ion mobility and reversibility. Although significant progress has been made in electrolyte design, the positive electrode remains a major bottleneck.[1]

To address this challenge, we developed a new family of cation-containing amorphous sulfonamide coordination polymers that serve as highly versatile positive electrode materials.[2] These frameworks reversibly store a broad range of divalent cations, including Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, and Zn^{2+}. They operate at high working potentials, up to 3.2 V vs Ca^{2+}/Ca and 2.8 V vs Mg^{2+}/Mg, while delivering fast kinetics, long-term cycling stability, and exceptionally low hysteresis. Importantly, they demonstrate the first reversible Sr^{2+} and Ba^{2+} storage, establishing a truly universal host for divalent ions. Their performance stems from the synergy between delocalized anionic charge, flexible and disordered cation coordination, and the structural adaptability of the amorphous framework. These features weaken metal-ion binding and promote rapid diffusion, enabling the storage of pure solid-state divalent ions without solvent or anion co-intercalation, an enduring challenge in the field.

Composed of earth-abundant, non-toxic elements, these coordination polymers combine sustainability with outstanding electrochemical performance. By merging inorganic robustness with organic flexibility in an amorphous structure, they define new design principles for next-generation divalent metal-ion batteries and challenge the high-voltage stability of current electrolytes, paving the way toward practical Mg- and Ca-based energy storage technologies.

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EES - D3 - F02
Chemical insights into triboelectric charging of polymers and organic powders

Bilge Baytekin[1], Niloofar Kamyar[1], Mahnam Ebadi[1], H. Tarik Baytekin[2], Erol Yildirim[2°]
[1]Bilkent University, TR; [2]Middle East Technical University, TR

Insulating materials readily acquire electrostatic charge through contact, and the slow relaxation of these charges poses persistent challenges in industrial processes. Common consequences include material adhesion, flow disruption, agglomeration, and particle segregation, while uncontrolled charge discharge may lead to hazardous events such as fires or explosions, resulting in millions of dollars in annual losses. Addressing these issues requires a deeper mechanistic understanding of triboelectric charge generation and decay. Chemical insight into these two events can help address the challenges mentioned.
But *why the polymer and organic molecular compound powders*?
We focus on triboelectrification of organic bulk polymers and molecular powder compounds because these materials constitute a major class of insulators widely encountered in industrial applications. All branches of industry, i.e., pharma, air and space, textiles, food, and plastics, suffer from the aforementioned detrimental effects of tribocharging. Although triboelectrification in these materials has been studied extensively, existing knowledge is largely based on empirical observations, and the underlying chemical mechanisms remain only partially resolved.
Then, *what chemical events occur during charge formation and dissipation*?
In this work, we systematically and comparatively analyze the triboelectric behavior of bulk polymers and organic molecular powders. We use different contact and charging modes (simple contact and tapping) to measure the charge under different environmental conditions (temperature and humidity). We analyze the materials for physical, chemical, and mechanical changes that may have occurred before and after charging to detect surface chemical changes. The results indicate that charge generation in polymers is primarily governed by bond scission and material transfer at contacting interfaces. In contrast, the electrification of organic powders is influenced by a broader set of parameters, including crystallinity, crystal structure, particle size, and intrinsic molecular properties such as ionization energy and electron affinity. Finally, the chemical structure and reactivity underlie the contact charging of all organic materials. We believe that energy losses can be mitigated and more sustainable processes can be achieved by addressing triboelectrification problems with greater chemical insight.

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EES - D3 - F03

Catalytic depolymerization of commercial grade polyurethane sponge using Ru- supported heterogeneous catalysts

Francesco Brandi[1]*, Carmen Moreno-Marrodán[1], Francesca Liguori, and Pierluigi Barbaro[1]*
[1]*Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti Organo Metallici, IT*

Background and motivation: Plastic waste accumulation in the environment is one main challenge for humanity. Among plastic, Polyurethanes (PU) are a class of specialty polymers with a vast array of applications and a global market volume expected to reach 28 Mton in 2025.[1] Nevertheless, PU recycling is still extremely challenging.[2] Catalytic chemical hydrogenolysis of PU is a promising approach in which PU are depolymerized to amines and polyols with the action of a redox catalyst. [2] Up to date, there are few examples of such approach in literature, mostly focusing on homogeneous catalyst (Ru, Mn, and Ir-pincer) with the addition of mineral bases.[3] In this work, we investigated the hydrogenolysis of a toluene di-isocyanate(TDI)-polyester commercial grade polyurethane sponge (Figure 1) using EtOH as a solvent and Ru/Al_2O_3 as heterogeneous catalyst.

Materials and methods: The reactions were carried out in autoclaves equipped with magnetic stirring and barometer for pressure reading. Typical reaction involved PU, Ru/Al_2O_3 catalyst and EtOH as a solvent. The reaction products have been quantified with GC-FID.

Results and discussion: Initially, Ru/Al_2O_3 was identified as the best catalyst at the optimum conditions of 250°C and 30 bar H_2 and selected to perform further investigations. The selected Ru/Al_2O_3 catalyst was used to depolymerize the TDI-polyester commercial sponge. The conversion was found quantitative with the alkyl di-esters (diethyl -glutarate, -adipate, and -succinate) as the major products (Figure 1). In addition to the diester, alkylated di-amines emerged as secondary by products. Overall, the cumulative monomer yield was measured of 51 wt.% compared to the initial PU sponge. Additionally, optimization of reaction parameter, such as Pressure, temperature and time, yielded in an optimum cumulative yield of 85 wt% at 225°C (Figure 2) In conclusion, this study demonstrated that heterogeneously catalyzed PU hydrogenolysis is a promising approach toward a plastic circular economy.

Acknowledgements: F.B. received funding from the European Union's Horizon Europe research and innovation program under the Marie Skłodowska-Curie (Grant agreement ID: 101207710). F.B. and P.B. thank the Circular and Sustainable Made in Italy (MICS) Extended Partnership, funded by the European Union Next-Generation EU (PNRR, Mission 4, Component 2, Investment 1.3 – D.D. 1551.11-10-2022, PE00000004) for funding. The project "Le materie prime del futuro da fonti non-critiche, residuali e rinnovabili" (FutuRaw), Fondo Ordinario Enti di Ricerca (D.M. 789, 2023), Ministero dell'Università e della Ricerca, Italy, is also gratefully acknowledged.

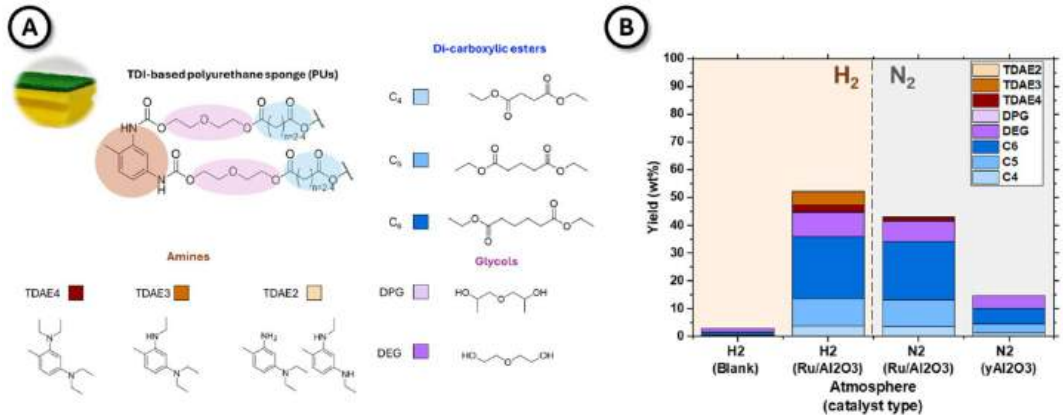

Fig. 1. A) Simplified structure of the PUs and structure of the identified and quantified PU depolymerization products grouped intro i) dicarboxylic acid esters, ii) amines, and iii) glycols. **B)** PU depolymerization products yield as a function of reaction atmosphere and catalyst type. Reaction conditions: m_{cat} = 20 mg, m_{PUs} = 100 mg, V_{EtOH} =10 mL, t = 17 h, T= 200 °C, r_{stir}=700 rpm, p_{system} = 10 bar H_2 or N_2

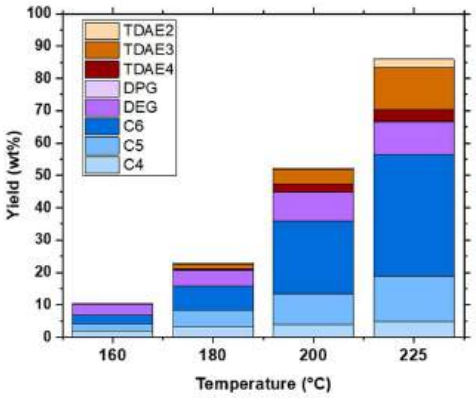

Fig. 2. PUs depolymerization products yield as a function of reaction temperature over Ru/Al_2O_3 catalyst. Reaction conditions: m_{cat} = 20 mg, m_{PUs} = 100 mg, V_{EtOH} =10 mL, t = 17h, T= 160, 180, 200 and 225°C, r_{stir}=700 rpm, p_{system} = 10 bar H_2.

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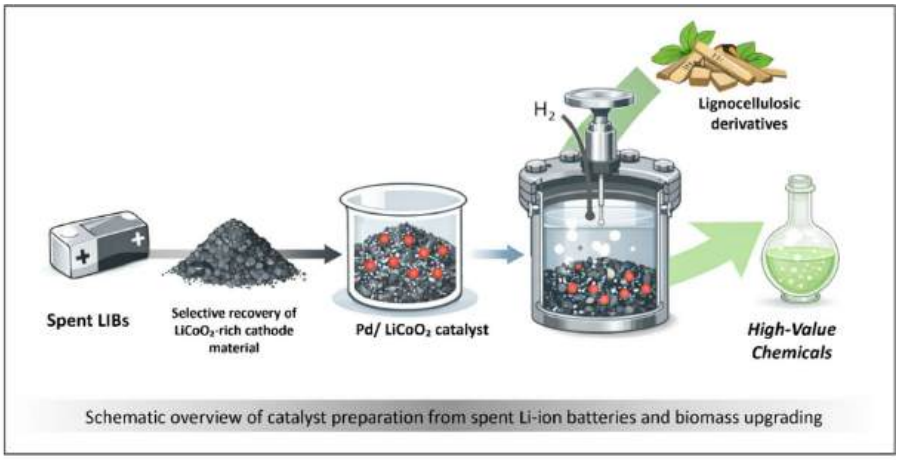
EES - D3 - F04

Waste Meets Waste: Upcycling Spent Li-Ion Battery-Derived Materials into Pd-Based Catalysts for Biomass Valorization

Giulia Maria Itri [1,2] , Francesco Mauriello [1], Andrea Donato [1], Tapio Salmi [3], Emilia Paone [1] .
[1] Università degli Studi Mediterranea di Reggio Calabria, IT, [2] Università degli studi di Perugia, IT, [3] Åbo Akademi University, FI

The rapidly increasing generation of electronic waste represents a major environmental and resource-related challenge, primarily due to the high content of critical and valuable metals in spent lithium-ion batteries (LIBs)[i]. At the same time, these waste streams offer a unique opportunity for valorization as promising heterogeneous catalysts or catalyst supports, enabling the direct reuse of complex metal-containing materials in chemical transformations. In this context, $Pd/LiCoO_2$ is investigated as an efficient and sustainable catalyst for the hydrogenation of furfural, a key platform molecule derived from lignocellulosic biomass residues. $LiCoO_2$ was selectively recovered from spent LIB cathodes through a simple mechanical separation and directly reused as a catalyst support, thereby avoiding complex and energy-intensive refining procedures. Palladium was introduced by impregnation, exploiting the beneficial role of a second metal in promoting strong metal–support interactions and synergistic effects. For instance, the addition of cobalt to palladium is helpful to enhance catalytic performance, including in hydrogenation reactions[ii].
The catalytic system was characterized by physicochemical techniques, revealing that the cobalt-containing $LiCoO_2$ matrix actively promotes intimate interactions with palladium, which play a decisive role in governing catalytic performance. As a result, the $Pd/LiCoO_2$ system exhibited high activity and selectivity in furfural hydrogenation, favoring the formation of furfuryl alcohol (FAL) and tetrahydrofurfuryl alcohol (THFA) under mild reaction conditions (150 °C, 6 h). Both products are valuable intermediates for the chemical and pharmaceutical industries[iii].



Schematic overview of catalyst preparation from spent Li-ion batteries and biomass upgrading

Overall, this work demonstrates a viable waste-to-catalyst strategy that effectively integrates e-waste valorization with biomass upgrading, providing a sustainable pathway toward the development of high-performance catalytic materials within a circular economy framework.

EES - D3 - F07

Synergistic Thermal and Stability Effects **of Al_2O_3–ZnO hybrid nanofluids in solar thermal collectors**

Jesús León-García[1], José Javier Delgado-Marín[1], Imane Moulefera[1], Ignacio Carnerero[1], Mercedes G. Montalbán[1], Gloria Víllora[1]

[1]Chemical Engineering Dept., Faculty of Chemistry, CEIR Campus Mare Nostrum (CMN), University of Murcia, ES

Renewable energy sources play a pivotal role in the transition towards a decarbonized and sustainable energy sector. However, conventional heat transfer fluids (HTFs), such as water or ethylene glycol, have limitations in thermal conductivity, heat capacity, and stability at high temperatures. In this context, improving energy efficiency and ensuring the sustainability of the global energy system are crucial, as well as developing new strategies to mitigate climate change [1].

Hybrid nanofluids (H-NFs) combining alumina (Al_2O_3) and zinc oxide (ZnO) nanoparticles were prepared in distilled water and examined as potential working fluids for flat-plate solar collectors (FPSC) [2]. Alumina (1 wt%) was kept constant while the mass of ZnO was varied from 0.25 to 1 wt.% [3], allowing the influence of the concentration of ZnO to be assessed in terms of thermal performance and colloidal stability. The characterization showed that the Al_2O_3 1%- ZnO 0.25 % H-NF displays the most consistent improvement, with a thermal conductivity increase of 23.4 % compared with the single-nanoparticle Al_2O_3 nanofluid and 71.5% relative to water, while preserving acceptable values of specific heat capacity and high stability. This H-NF was then evaluated in a thermal flat-plate solar collector and compared directly with water under three operating flow rates (Figure1). The collector tests revealed a clear difference in thermal response: the H-NF reached a maximum temperature rise of approximately 5 °C, whereas water achieved 3.4 °C under the same conditions, corresponding to a 46.8% higher temperature gain. These trends suggest that the enhanced conductivity plays a dominant role in heat uptake at low to moderate flow conditions.

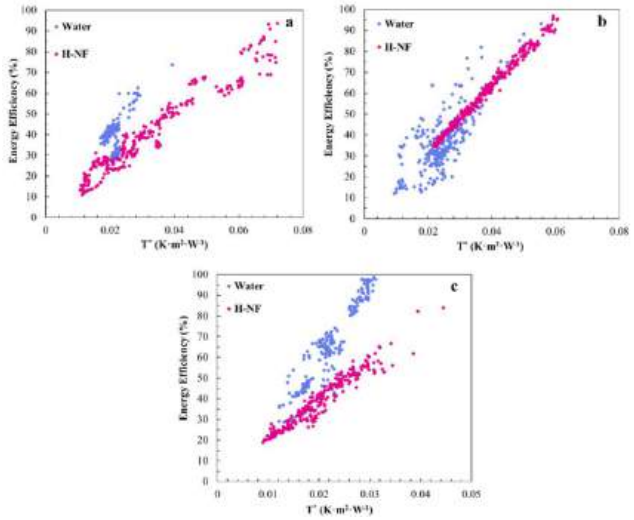


Fig. 1.*Thermal energy efficiency of the FPSC at flow rate of; a) 6.12 L/h; b) 12.40 L/h and c) 24.48 L/h.*

Funding: This work is part of the following research projects: Ref. PID2023-150761OB-C21 funded by MICIU/AEI/10.13039/501100011033 and by FEDER, UE and Ref. 22129-PI-22 funded by the research support program of the Seneca Foundation of Science and Technology of Murcia, Spain. J.J. Delgado-Marín acknowledges support from the *Juan de la Cierva* contract (Ref. JDC2023-052774-I) funded by MICIU/AEI /10.13039/501100011033 and the FSE+.

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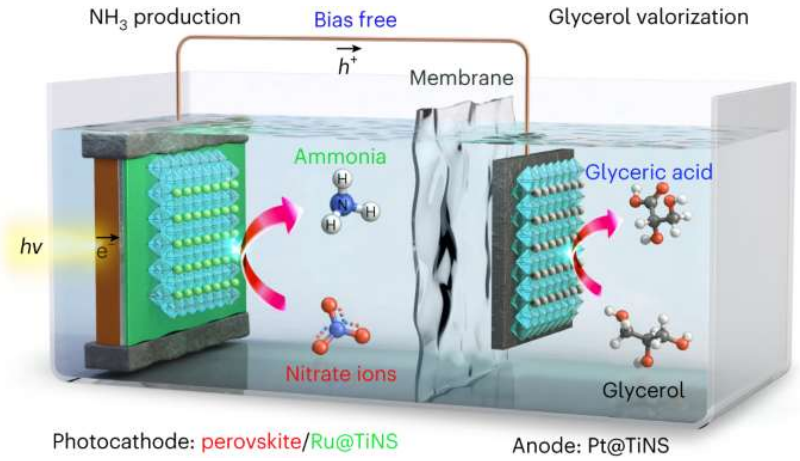
EES - D3 - F08
Photoelectrochemical solar ammonia production

Ahmad Tayyebi[1], Maria del Carmen Giménez-López[1]
[1]Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Universidade de Santiago de Compostela, ES

As an indispensable feedstock for fertilizers and chemicals, ammonia (NH_3) is predominantly synthesized via the Haber-Bosch process—a reaction demanding extreme temperatures and pressures that account for ~1% of global energy use and 1.6% of CO_2 emissions. Photoelectrochemical (PEC) conversion of nitrate to NH_3 presents a compelling renewable alternative, yet its development is constrained by two principal limitations: insufficient solar-to-ammonia productivity (SAP) and the high overpotentials required to sustain the overall redox process. For PEC NH_3 production to attain practical relevance, performance metrics must advance beyond current thresholds, specifically targeting production rates >1,000 μg_{NH3} cm^{-2} h^{-1}.
PEC ammonia synthesis presents a sustainable pathway to decarbonize the NH_3 value chain. However, the overall efficiency of conventional PEC systems is limited by the significant external bias required to drive the coupled anodic oxygen evolution reaction (OER) alongside cathodic nitrate reduction. This presentation will examine and compare various solar-driven approaches for ammonia production, including integrated PEC, photovoltaic-electrochemical (PV-EC), and self-biased (unbiased) PEC systems. Furthermore, we propose a strategy to enhance both the energy and economic efficiency of this process by replacing the OER with a thermodynamically more favorable, value-added organic oxidation reaction. This hybrid anodic process not only reduces the total cell voltage but also enables the co-production of economically valuable chemicals, creating an integrated system for simultaneous wastewater valorization and green ammonia synthesis.



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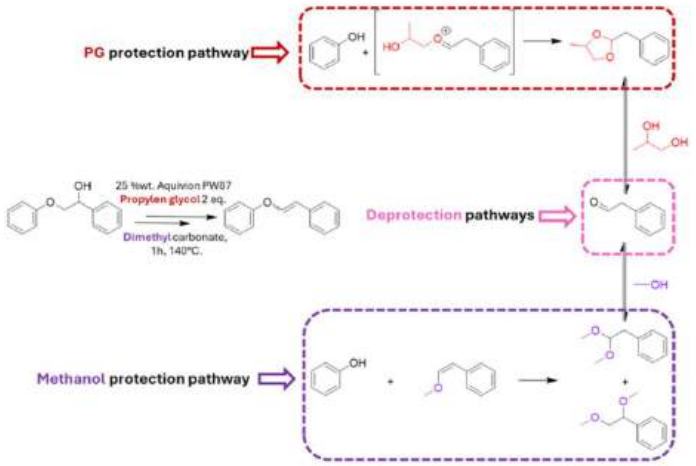
EES - D3 - F09

Lignin acidolysis via a βO4 model compound: An improvement based on heterogeneous superacid catalysis

Giuseppe Salierno[1], Federico Bugli[1], Ilaria Bonora[1], Francesco Mauriello[2], Emilia Paone[2], Tommaso Tabanelli[1]
[1]University of Bologna, "Toso Montanari" Dept. of Industrial Chemistry, IT; [2]Università Mediterranea di Reggio Calabria, Dipto DICEAM, IT

The valorization of the lignin fraction of lignocellulosic biomass remains a major bottleneck in the development of economically viable and sustainable biorefineries. State-of-the-art approaches such as Reductive Catalytic Fractionation (RCF) have demonstrated remarkable selectivity toward valuable phenolic monomers. [1] However, their reliance on noble-metal-based catalysts (e.g., Ru, Pd) significantly increases process costs and raises concerns regarding scalability and long-term feasibility. In this context, K. Barta et al.[2,3] demonstrated that acid-catalyzed solvolysis represents a promising metal-free alternative. The strategy developed is based on the solvolysis of a lignin model compound in dimethyl carbonate (DMC) followed by acidolysis using a homogeneous acid catalyst and stabilizing reactive intermediate with ethylene glycol. Building on this approach, we advanced toward a greener process by adapting homogeneous catalysis with a heterogeneous system. Different solid acid catalysts namely Aquivion PW87 and Amberlyst 15 were investigated for the acidolysis of 2-Phenoxy-1-Phenylethanol (2P1P) in DMC, suppressing the recondensation using propylene glycol (PG) to generate reversible acetal species. Notably, methanol formed in situ from DMC also actively participates in intermediate stabilization. Although both resins exhibit strong acidity, the investigated catalysts displayed markedly different stability under mild conditions. Additional insights were gained regarding both the reaction scheme, supported by targeted experiments on key reaction intermediates, and the influence of the protective group chain length.

Fig. 1. Different protection pathways of Aquivion PW87 catalyzed cleavage of 2P1P using PG as protective group in DMC as solvent.



Acknowledgments: Financed by the European Union - NextGenerationEU through the Italian Ministry of University and Research under PNRR "Piano Nazionale di Ripresa e Resilienza" - Mission 4 "Istruzione e Ricerca" Component 2 "Dalla ricerca all'impresa", Investment 1.1, "Fondo per il Programma Nazionale di Ricerca e Progetti di Rilevante Interesse Nazionale (PRIN) – Piano Nazionale di Ripresa e Resilienza, addressed to Progetti di Ricerca di Rilevante Interesse Nazionale". "ENCAPSULATE" codice2022KTAH2L - CUP: J53D23007620006.

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EES - D3 - F10
Innovative heterobimetallic precursors for multifunctional fluoride materials

Claudia Barbagallo[1,2], Francesca Lo Presti[1,2], Anna L. Pellegrino[1,2], Graziella Malandrino[1,2]
[1]Dipto di Scienze Chimiche, Università degli Studi di Catania, IT; [2]INSTM UdR Catani, IT

In the last decades, fluoride-based materials are considered promising systems for several technological applications, as optics, sensors and photovoltaics[1]. In particular, binary and ternary lanthanide-based fluoride films, doped with rare-earth ions, have been employed in solar cells. These materials enhance the efficiency of photovoltaic systems[2] since they are able to absorb a wider portion of solar energy spectrum. Generally, energy conversion layers require an inorganic fluoride matrix based on alkaline metals, such as sodium, and a luminescent element like europium[3-4].
Besides, luminescent species-doped fluoride systems can be used for the detection of polluting species such as nitro-aromatic compounds.
In this study, the synthesis of innovative cesium-based metalorganic complexes containing rare earth metals is reported. The precursors show high stability, interesting thermal properties, such as high volatility and good mass transport properties, and high solubility in ethanol that make them valid candidates for vapor and solution deposition approaches of fluoride-based functional materials.
The present work describes an efficient one-pot synthesis of two novel bimetallic adducts based on cesium-yttrium or cesium-europium, using β-diketonate ligands and polyethers. The structures of Cs(I) metal-organic compounds is "$CsRE(hfa)_4 \cdot 2$tetraglyme", with RE = Y(III) or Eu(III), Hhfa = 1,1,1,5,5,5-hexafluoro-2,4-pentanedione and tetraglyme = 2,5,8,11,14-pentaoxa-pentadecane.
These compounds have been characterized in terms of structural and thermal properties.
Through a sol-gel process, Cs-RE-fluoride layers have been obtained from these precursors.
In addition, cesium-europium film shows intriguing features to be employed as a sensor to determine the presence of nitro-compounds in water-based solutions, based on the luminescent properties of the lanthanide element.

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EES - D3 - F11

Novel molecular and polymersome-based systems for photocatalytic CO_2 reduction, towards compartmentalized artificial photosynthesis

Carla Casadevall[1,2,*], Laura Velasco-Garcia[1,2], Edelman J. Espinoza-Suárez[1,2], Akhmet Bekaliyev[1,2], Leonardo Quesada-Román[1,2]

[1]Dept. of Physical and Inorganic Chemistry, University Rovira i Virgili (URV), ES; [2]Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, ES

The sustainable synthesis of fuels and chemicals using sunlight as driving force and simple readily available feedstock such as H_2O and waste CO_2 provides a potential feasible pathway to mitigate increasing CO_2 emissions and transitioning toward a greener chemical industry. In this context, natural photosynthesis is a source of inspiration and has led to the evolving and multidisciplinary field of artificial photosynthesis (AP).[1-4] However, when designing bioinspired photocatalytic platforms for AP, the compartmentalization found in nature is sometimes overlooked. Our research group is currently studying how this key structural ffeature can be translated to develop bioinspired artificial photocatalytic systems.[4] We are working in the development of polymersomes functionalized with (photo)catalysts to produce solar fuels and chemicals in aqueous media using solar energy as driving force.[5] We have developed a novel family of asymmetric porphyrin and phthalocyanine complexes bearing Co, Ni, and Fe as 1st row transition metal centers for photocatalytic CO_2 reduction (CO_2R) in combination with Ir- and Cu-based photosensitizers and organic photosensitizers, under visible light irradiation (447 nm) in aqueous-organic mixtures in presence of a sacrificial electron donor.[5,6] The Co, Fe and Ni phthalocyanine complexes show a remarkable photocatalytic activity and selectivity for photocatalytic CO_2R to CO in homogeneous conditions, even with 10% of water. In contrast, the porphyrin complexes show remarkable activity and selectivity for methane production. Moreover, to further explore the applicability and increase the stability of these systems, we have anchored both the CO_2R catalyst and photosensitizer onto the membrane of polymersomes, developing the first polymersome for compartmentalized photocatalytic CO_2R.[5] The effect of anchoring and the nature of the photosensitizer used allows to tune the selectivity of the photocatalytic reaction to obtain only CO_2R derived products in water, suppressing the normally competing hydrogen evolution reaction. Mechanistic studies are ongoing to rationalize these differences in reactivity between homogeneous and heterogenized systems.

The authors thank the Spanish Ministry of Science, Innovation, and Universities for the “Ramón y Cajal” contract (ref: RYC2021-030935-I, C.C.), the Knowledge Generation Project (PID2022-142975OA-I00, C.C.), and the Severo Ochoa Excellence Accreditation (CEX2019-000925-S, MIC/AEI). We also thank the European Union for an ERC Starting Grant (ERC-StG-2025, BIOPOLE, 101222089) and the 2024 Leonardo Grant (BiPolPhotoCO2) for Researchers and Cultural Creators, from the BBVA Foundation, which the author thank. The BBVA Foundation accepts no responsibility for the opinions, statements, and contents included in the project and/or the results thereof, which are entirely the responsibility of the authors.

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EES - D4 - O01

Enhancing low-temperature CO_2 methanation via nickel electronic structure engineering

Bing Bai[1,2], Bert M. Weckhuysen[1]

[1]Inorganic Chemistry and Catalysis Group, Institute for Circular and Sustainable Chemistry, Dept. of Chemistry, Faculty of Science, Utrecht University, NL

CO_2 hydrogenation to methane (Sabatier reaction) plays a central role in carbon valorization and renewable hydrogen storage within Power-to-X energy systems. However, conventional Ni-based catalyst materials generally suffer from a critical trade-off: high catalytic activity is typically achieved only at elevated reaction temperatures above 400 °C, leading to substantial energy consumption, whereas at lower temperatures their performance is severely limited by strong adsorption of reaction intermediates, such as formate and CO, which causes active-site blocking (Figure 1). Overcoming intrinsic limitation is essential for realizing an energy-efficient, low-temperature CO_2 methanation, which has been a core research topic in the past years.

In this work, manganese oxide (MnO_x) is identified as a highly efficient promoter that addresses this challenge through a deliberate engineering of the electronic structure of Ni. On both inert Al_2O_3 and reducible CeO_2 supports, MnO_x establishes an intimate interfacial contact with Ni nanoparticles, inducing directional electron transfer from Ni to MnO_x. This interaction retards the reduction of NiO and stabilizes Ni in a partially oxidized state ($Ni^{\delta+}$) rather than a fully metallic Ni^0. Such electronic modulation effectively weakens the adsorption strength of formate and CO intermediates on Ni sites, suppressing their accumulation and facilitating sequential hydrogenation and desorption steps, thereby alleviating active-site blockage. In addition, MnO_x introduces redox-active Mn^{4+}/Mn^{2+} couples that promote CO_2 activation and enhance Ni dispersion, maximizing the number of accessible active sites. Owing to these synergistic effects, the optimized $Ni/6MnO_x/CeO_2$ catalyst delivers 80.7% CO_2 conversion at ~ 250 °C, along with a 28-fold increase in methane space-time yield compared to an unmodified Ni/CeO_2 (Figure 2).

This study establishes a generalizable design principle for low-temperature CO_2 methanation catalysts centered on Ni electronic structure engineering, offering a practical strategy to reduce the energy footprint of CO_2 valorization and to advance its integration into sustainable Power-to-X energy conversion technologies.

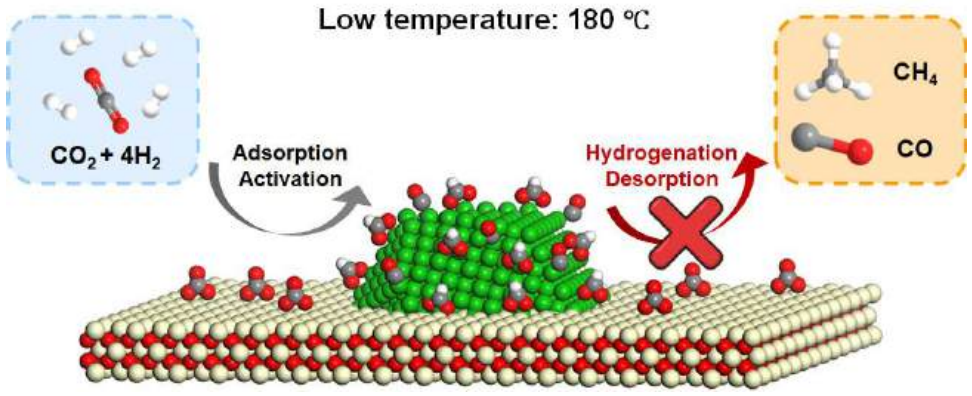

Fig. 1. Low-temperature Ni-based catalysis is limited by strong intermediate (i.e., HCOO* or CO*) adsorption that blocks active sites and inhibits CH_4 formation despite efficient CO_2 activation.

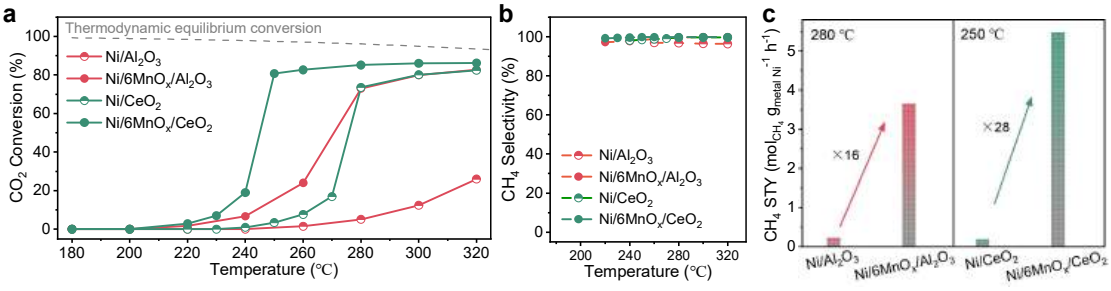

Fig. 2. Catalytic Performance of $Ni/nMnO_x$/Support Catalysts in CO_2 Hydrogenation. (a) CO_2 conversion, (b) CH_4 selectivity, and (c) low-temperature catalytic activity comparison.

Acknowledgements: The authors gratefully acknowledge Utrecht University, including its technical staff, for their valuable support, including financial resources.

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EES - D4 - O02

Solar-driven CO_2 to methanol production

Natalia Mazur[1], Alexia Magni[1], Dimitrios Drettas[1], Jelle Rohlfs[1], Jonathan van den Ham[1], Nicole Meulendijks[1], Pascal Buskens*[1, 2], Francesc Sastre*[1,3]

[1]The Netherlands Organisation for Applied Scientific Research (TNO), NL; [2]Institute for Materials Research (imo-imomec), DESINe Group, Hasselt University, BE; [3]Instituto de Tecnología Química Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Universitat Politècnica de València, ES

Solar-driven CO_2 reduction has attracted increasing attention within the Carbon Capture Utilization (CCU) technologies as a strategy to transform CO_2 into value-added products while simultaneously storing intermittent renewable energy.[1] The main reported products of plasmonic CO_2 reduction are CO and CH_4. [2-6] However, methanol is a particularly attractive product because it is liquid under ambient conditions, which facilitates storage and transport, and it serves as a versatile platform molecule for the synthesis of higher-value chemicals. Current industrial methanol production remains largely dependent on fossil-derived feedstocks, primarily via methane steam reforming. Developing selective catalytic process that directly utilize CO_2 as a carbon source is of a significant technological and environmental importance.

Methanol synthesis from CO_2 is an exothermic and equilibrium-limited reaction. Elevated temperatures shift the reaction toward the competitive reverse Water gas shift (rWGS) reaction, however substantial energy input is required to activate the CO_2 molecule. To overcome these limitations, we investigated the solar-driven methanol production using plasmonic Cu nanoparticles supported on ZnO and promoted with Al_2O_3 (CZA), as a plasmonic catalyst to enhance the light harvesting, and methanol production rate.

The Al_2O_3 promoter content plays a critical role in enhancing the methanol production rate and product selectivity. Systematic variation of the Al_2O_3 loading from 0.5% to 20 % shows that methanol production reaches a maximum at 12 % Al_2O_3, with the production rate declining at higher loadings as shown in Figure 1.

These findings demonstrates that the CZA plasmonic catalyst can efficiently drive the direct CO_2 to methanol reaction under mildly concentrated solar irradiation, offering a promising route towards sustainable, sunlight-driven methanol production.

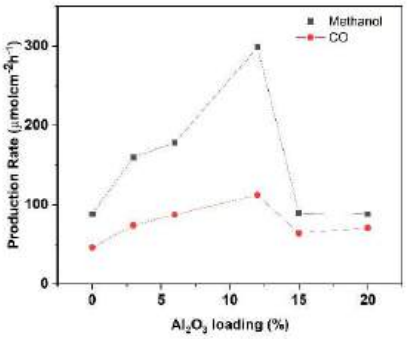

Fig. 1. Methanol and CO production rate as a function of the Al loading under 25 suns irradiation without conventional reactor heating

Acknowledgements: This work received funding from the European Union's the EC Interreg Flanders-The Netherlands project FOTON, www.projectfoton.nl.

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EES - D4 - O03
Engineering biopolymeric adsorbents with ionic liquids for efficient CO_2 capture

José Javier Delgado-Marín[1], Jesús León-García[1], Imane Moulefera[1], Ignacio Carnerero[1], Mercedes G. Montalbán[1], Gloria Víllora[1]
[1]*Chemical Engineering Department, Faculty of Chemistry, CEIR Campus Mare Nostrum (CMN), University of Murcia, ES*

The continuous rise in atmospheric CO_2 is one of the main contributors to global warming, making the development of efficient and sustainable capture materials critically important. Biopolymer-based adsorbents offer a promising alternative to conventional systems due to their renewability, low toxicity, and ease of functionalization [1].
In this study, the CO_2 adsorption behavior of four biopolymeric substrates, microcrystalline cellulose (C), chitosan (Q), cellulose nanoparticles (NPC) and silk fibroin nanoparticles (SFN), was evaluated after surface modification with selected ionic liquids (ILs). The adsorption profiles shown in Figure 1 reveal clear differences related to substrate type and IL treatment. Among all materials, SFN-[Col][Oct] displayed the highest CO_2 uptake, characterized by a fast rise in the adsorption curve followed by a stable plateau [2]. This improvement may be due to the high surface area of SFN and the strong interactions between the IL and the functional groups of the protein, which enhance the accessibility of active sites. NPC-[Col][Oct] also showed a noticeable increase in CO_2 adsorption compared to untreated NPC, although its performance remained below that of SFN. In contrast, microcrystalline cellulose and chitosan presented lower adsorption capacities. Their IL-modified forms showed only moderate improvements, likely due to their more compact structures and the limited availability of surface binding sites. These observations highlight the strong influence of morphology, porosity, and IL distribution on adsorption performance. Overall, the results demonstrate that IL treatment is an effective strategy to enhance CO_2 adsorption in biopolymeric materials. The combination of ILs with nanostructured substrates, particularly SFN and NPC, appears especially promising for the development of greener and more efficient CO_2 capture technologies.

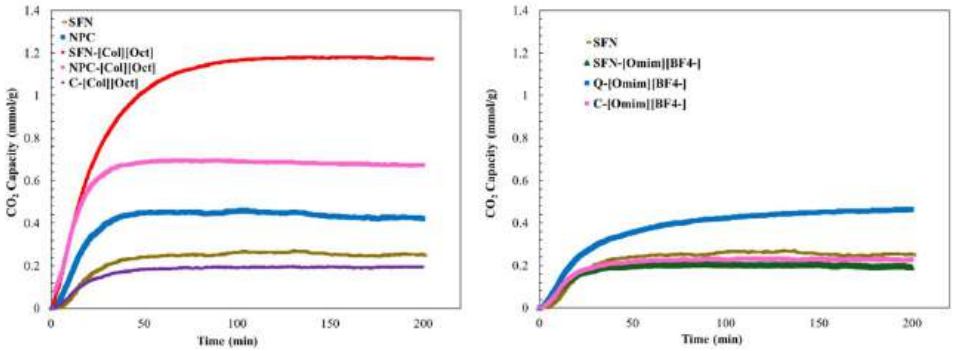

Fig. 1. CO_2 Adsorption Profiles of IL-Modified Biopolymeric Substrates (C, Q, NPC, and SFN).

Funding: This work is part of the following research projects: Ref. PID2023-150761OB-C21 funded by MICIU/AEI/10.13039/501100011033 and by FEDER, UE and Ref. 22129-PI-22 funded by the research support program of the Seneca Foundation of Science and Technology of Murcia, Spain. J.J. Delgado-Marín acknowledges support from the *Juan de la Cierva* contract (Ref. JDC2023-052774-I) funded by MICIU/AEI /10.13039/501100011033 and the FSE+.

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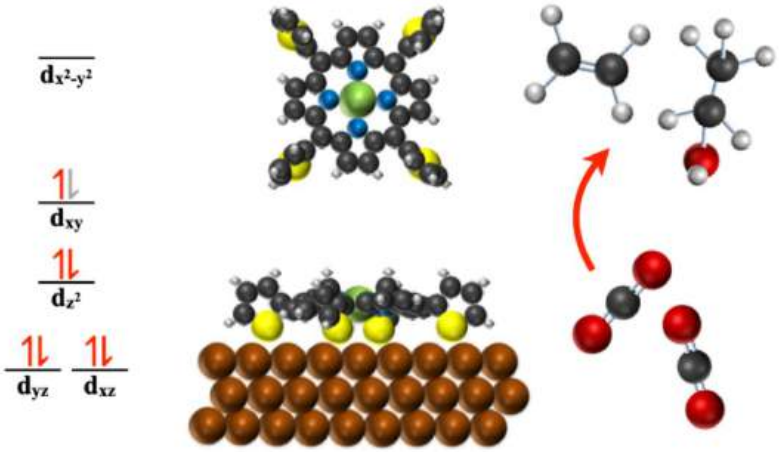
EES - D4 - O04
Model thiophene-decorated nickel porphyrins for tandem CO_2 reduction

Sung-Fu Hung[1]
[1]Dept. of Applied Chemistry and Center for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, TW

Tandem systems that integrate CO-generating catalysts with copper have shown promise for enhancing CO_2RR performance. Sulfur-containing single-atom catalysts (SACs) are particularly effective for CO production;[1] however, the role and positioning of sulfur in facilitating both CO_2-to-CO conversion and tandem CO_2RR remain elusive. Here we show model thiophene-decorated nickel porphyrins as model SACs that exhibit tandem activities in CO_2RR.[2] Spectroscopic and theoretical analyses reveal that thiophene substituents induce ligand holes, regulating the d orbitals and d-band center of the nickel center to reduce the reaction barrier and promote CO formation. Coupling these SACs with a copper catalyst achieves a Faradaic efficiency of 74.3% and a partial current density of 445.8 mA cm^{-2} for C2 products in a neutral solution—a 46% improvement over bare copper. *Operando* studies confirm the formation of CO intermediates from the SACs, highlighting their role in facilitating tandem catalysis.

The supports from the National Science and Technology Council, Taiwan (Contract No. NSTC 113-2628-M-A49-008 and NSTC 114-2628-M-A49-005) are gratefully acknowledged. We also thank the support from the Yushan Young Scholar Program (MOE 114-YSFMS-0010-003-P2) and the Center for Emergent Functional Matter Science, Ministry of Education, Taiwan. This work was supported by the Higher Education Sprout Project of the National Yang Ming Chiao Tung University and Ministry of Education (MOE), Taiwan.



Scheme for thiophene-decorated nickel porphyrins for tandem CO_2 reduction

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EES - D4 – O05

Microcrack-engineered gas diffusion layers to mitigate flooding in Zero-Gap CO_2 electrolysers for CO production

Thijs Van Thillo[1*], Luis F. Leon-Fernandez[1], Tom Breugelmans[1]
[1]Research Group Applied Electrochemistry and Catalysis, University of Antwerp, BE

Electrolysers show great promise to decarbonise industry by storing renewable electricity in energy-dense chemicals and upgrading low-value feedstocks such as CO_2 [1]. In particular, CO2 electrochemical conversion to CO—a key building block for numerous energy-dense compounds—stands out as a potential route towards the profitability levels of fossil-based industrial counterparts [1].
However, there are challenges to overcome before CO_2 electrolysers reach efficiencies acceptable for industrial deployment, including efficient delivery of gaseous reactants to the active sites. While zero-gap reactors can potentially minimise ohmic losses; in practice their operation is hindered by flooding of the electrode [2]. As a result, they rely heavily on hydrophobic gas diffusion layers (GDLs), which prevent electrolyte penetration beyond the catalyst layer. On the other hand, it has been reported that microcracks in the GDL formed during the manufacturing limit flooding by creating preferential water pathways [2].
This work aims to elucidate how GDL surface cracking influences CO_2 electrolyser performance in zero-gap configurations. Firstly, we study the effect of cracks on reactor performance by comparing two commercial GDLs: a crackless Freudenberg H23C6 and a cracked Sigracet 39BB (Fig. **2**a). Secondly, an engineered GDL (Fig. **2**b) is produced by femtosecond laser ablation of the crackless Freudenberg H23C6. Laser ablation allows us to create grooves that simulate the beneficial microcracks in a controlled manner.
Overall, in this work I will present the importance of engineering ordered microcracks—i.e., their density and geometry—to optimise CO_2 delivery and electrolyte supply without inducing flooding.

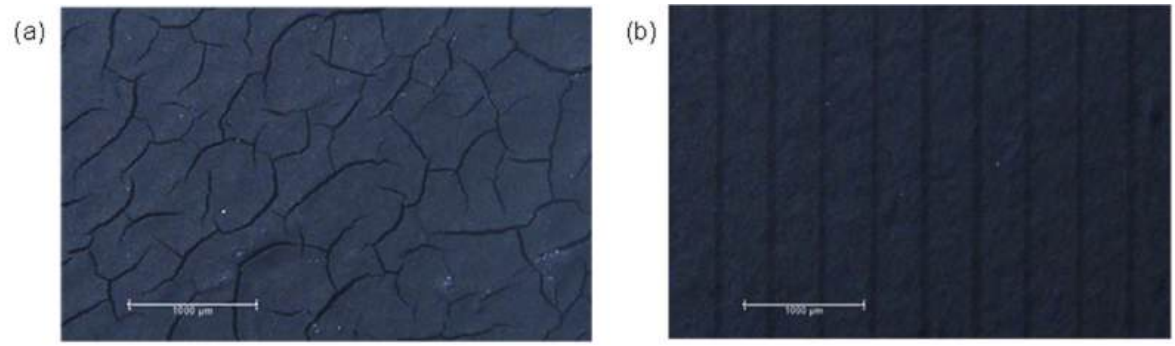

Fig. 2. Optical light microscope images of GDL surfaces: a) Sigracet 39BB with natural crack formation b) laser modified surface of Freudenberg H23C6

This work is part of the ERC research project TRANSCEND (Grant ID: 101088063).

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EES - D4 – O06

Benchmarking commercial anion exchange membranes for CO_2 electroreduction to ethylene

Natalia Mazur[1], Bernadetha Efata Ferryka[2], Dominick Clancy[3], Francesc Sastre[1,4]

[1]The Netherlands Organisation for Applied Scientific Research (TNO), NL; [2]Helmholtz Centre for Environmental Research (UFZ), DE; [3]University of Queensland, AU; [4]Instituto de Tecnología Química Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Universitat Politècnica de Valencia, ES

The electrochemical reduction of carbon dioxide (CO_2RR) in alkaline setting shows potential for revalorising CO_2 emissions and generating value-added chemicals such as ethylene. Within this context, the anion exchange membrane (AEM) plays a pivotal role, significantly influencing reaction rate, cell stability, product selectivity and ion transport. Regardless of the importance of the membrane, there is a lack of systematic comparison of commercially available AEMs for CO_2RR to ethylene under identical operating conditions.

In this study, 10 commercial AEMs were benchmarked using a zero-gap electrolyser, equipped with a Cu-based cathode, Ni-based anode and 1M KOH as anolyte. The performance of each membrane was evaluated across 3 current densities (50, 100, and 200 mA/cm^2), with key metrics including total cell potential, gas product distribution, and ion crossover.

The results reveal a strong correlation between the chemical and mechanical properties of the membranes, product selectivity and operational stability. Notably, membrane's mechanical properties such as thickness and mechanical reinforcement were found to have a considerable impact on cell potential and product selectivity expressed as faradaic efficiency. Membranes thicker than 60 µm and with reinforcement led to higher cell voltages and favoured the competing hydrogen evolution reaction. Membranes of intermediate thickness (30–60 µm) predominantly favour CO formation. Finally membranes thinner than 30 µm were particularly effective at promoting ethylene production over prolonged time periods. This favourable behaviour observed in thinner membranes is attributed to improved ion conductivity, as a result of efficient water management, which in turn limited cathode deactivation.

This systematic comparison demonstrates that the chemical and mechanical properties of AEMs play a crucial role in determining both the efficiency of CO_2RR and the selectivity towards desired products. These findings offer recommendations for the selection and development of AEMs to optimise CO_2RR to ethylene, and provide direction for future membrane development.

EES - D4 - O07

Research on electrocatalyst design and electrolyzer scaling for efficient CO_2 electroreduction

Jiaqi Feng[1], Xiangping Zhang[1]
[1]*China University of Petroleum-Beijing, CN*

The green electricity-driven electrochemical reduction of CO_2 to high-value-added chemicals not only facilitates carbon resource recycling but also promotes the low-carbon transition of energy-intensive industries. Focusing on the design of non-precious metal catalysts and the scaling-up of electrolysis systems, we have proposed a novel strategy utilizing rare-earth element modulation in copper-based catalysts to enhance the activity for multicarbon (C_{2+}) product formation. It was found that gadolinium (Gd) doping can suppress the hydrogen evolution reaction, provide moderate intermediate binding energy, and thereby promote C_{2+} generation. Furthermore, Gd doping induces lattice distortion in cuprous oxide, significantly accelerating the kinetics of carbon-carbon coupling and increasing C_{2+} selectivity by over 30%.[1] By further coupling the physical confinement effect of pore channels with the rare-earth doping strategy, we developed a new approach to strengthen CO_2 electroreduction to C_{2+} products in strongly acidic media. The physical confinement alters ion diffusion behavior on the catalyst pore surface, while rare-earth doping promotes carbon-carbon coupling. This catalyst achieves a C_{2+} product selectivity of 86% at a current density of 0.9 A cm^{-2} in an acidic electrolyte, with a single-pass CO_2 conversion of up to 80%.[2] Additionally, we designed and synthesized an unsaturated-coordinated manganese single-atom catalyst. The unsaturated coordination structure effectively lowers the free energy of key intermediate formation, facilitating CO production. When combined with an ionic liquid electrolyte, the high-selectivity window is significantly broadened.[3,4] Based on this, a universal strategy was developed for preparing unsaturated-coordinated single-atom catalysts using metal-containing ionic liquids as precursors. The catalyst was applied in a self-designed and constructed scaled-up electrolyzer system integrated with an ionic liquid electrolyte, enabling efficient conversion of CO_2 to syngas.

Acknowledgements: National Natural Science Foundation of China (22578491), Science Foundation of China University of Petroleum-Beijing (2462023BJRC034)

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EES - D4 - O08
Electrochemical hydrogenation using dispersed catalytic particles

Michael E. Reid[1], Alexander G. Holton[1], Louis C. Morrill[2*], Marc Pera Titus[1*]
[1]Cardiff School of Chemistry, Cardiff Catalysis Institute, Translational Research Hub, Cardiff University, UK;
[2]Dept; of Chemistry, University of Bath, UK

Hydrogenation is widely used in industry but traditional catalytic methods is carried out thermally using H_2,[1] which creates safety and handling challenges. Electrochemical hydrogenation (ECH) offers a greener alternative; yet many current approaches rely on modified electrodes, homogeneous catalysts, or toxic reductants, complicating scalability and sustainability.[2] In contrast, catalytic particles dispersed in electrolyte provide a simple, modular and recyclable platform, yet particle-catalyzed ECH has mostly been confined to aqueous electrolyte, divided-cell setups, restricting substrate scope.[3] The limited scope of the literature underscores a clear opportunity to extend particle-catalyzed ECH approaches to more complex organic transformations under non-aqueous electrolyte.
Herein, we investigate the ECH of diverse organic functionalities using commercial 5 wt% Pd/Al_2O_3 catalytic particles in an organic electrolyte. This approach enables efficient ECH of mono-, di-, tri-, and tetrasubstituted alkenes, as well as mono- and disubstituted alkynes, in addition to electrochemical dehalogenation of aryl halides, encompassing 50 examples with yields of up to 92%. Scalability was demonstrated, enabling product isolation on the gram scale. Mechanistic studies were conducted to probe both anodic and cathodic processes. Deuterium labelling experiments elucidated the hydrogen source during reduction, while catalyst–electrode interactions were examined using cyclic voltammetry, electrochemical impedance spectroscopy, double-layer capacitance, and zeta potential measurements. Furthermore, the recyclability of the catalytic system was evaluated, demonstrating that the reaction can be performed over multiple cycles without a significant loss in product yield. Collectively, these results highlight the versatility, scalability, and recyclability of our methodology, offering a more sustainable platform for organic synthesis by removing reliance on H_2 and reducing system complexity.

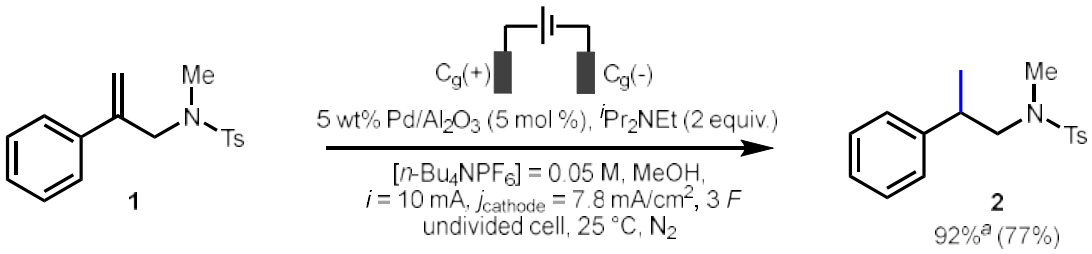

Fig. 1. Optimized reaction conditions for ECH of **1** using 5 wt% Pd/Al_2O_3 catalytic particles, $^{i}Pr_2NEt$ as a sacrificial reductant, in organic electrolyte (tetrabutylammonium hexafluorophosphate in methanol). [a] Determined by ^1H NMR analysis of the crude reaction mixture with 1,3,5-trimethylbenzene as the internal standard. Isolated yield is given in parentheses.

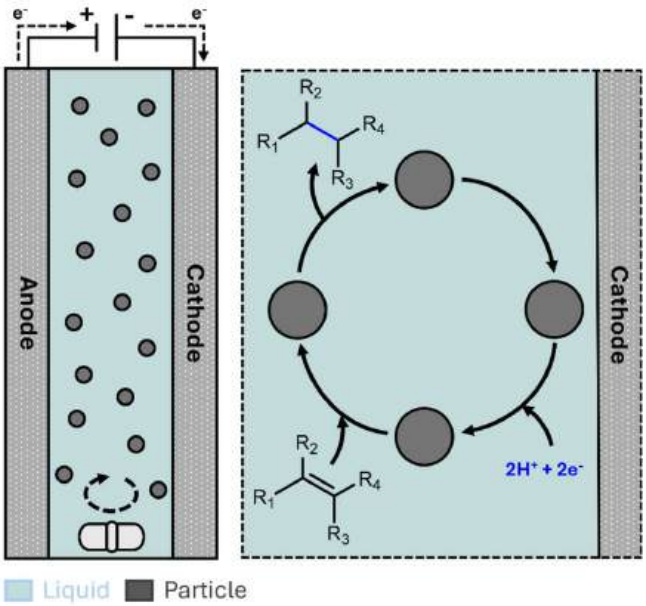

Fig. 2. Generalized scheme of our electrochemical particle-catalyzed hydrogenation of alkenes.

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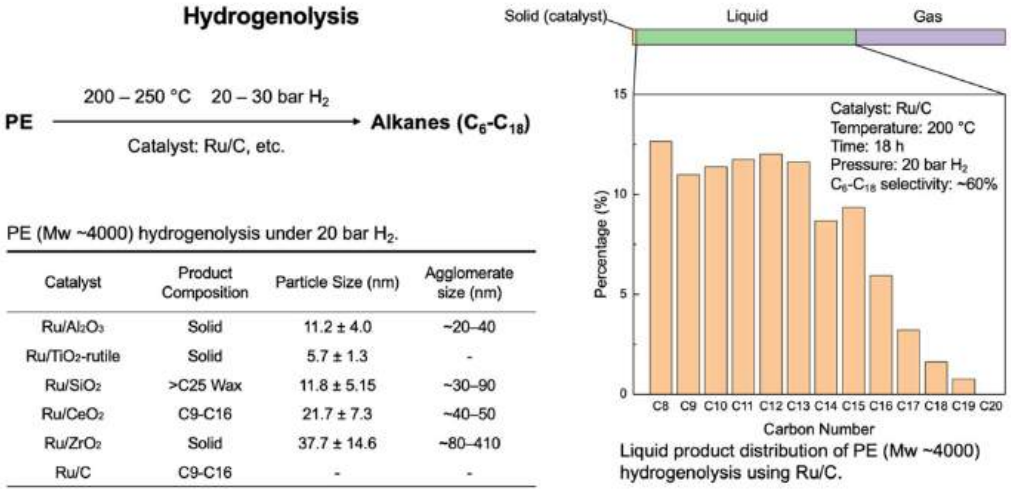
EES - D4 - O09
Development of catalyst systems for polyethylene recycling by hydrogenolysis

Haoxiang Yan[1], Florian Meirer[1]*, Bert Weckhuysen[1]*
[1]*Institute for Sustainable and Circular Chemistry, Utrecht University, NL*

Plastic pollution threatens ecosystems due to increasing plastic use and environment leakage. Polyethylene (PE) is among the most widely used plastics, with only ~12% recycled.[1] ACTPAC project aims to develop a complete path to convert PE first into alkanes, then into high-value chemicals (monomers) via bio-based processes, and finally produces fully biodegradable polyesters.[2] Within this consortium, Utrecht University is developing catalyst systems for selective PE hydrogenolysis to C_6-C_{18} hydrocarbons as monomers for next procedure. Ru/C was tested for the hydrogenolysis of PE, LDPE, HDPE, LLDPE, and UHMWPE under various conditions (200-250 °C, 20 bar H_2), delivering ~60% C_6-C_{18} selectivity for PE (Mw ~4000). Higher temperatures and longer reaction shifted product distribution toward lower-carbon-numbers. At 200°C and 20 bar H_2, PE, HDPE, and LLDPE showed higher selectivity towards liquid products, LDPE forms wax-like and gas products, while UHMWPE produces only gas at a longer reaction time. We further investigated Ru supported on Al_2O_3, TiO_2, SiO_2, CeO_2, and ZrO_2. Among these, Ru/CeO_2 showed highest selectivity towards C_6-C_{18} alkanes, achieving ~53% selectivity in this fraction. In contrast, Ru/SiO_2 showed lower activity, producing mainly C_{25}-C_{40} wax, while the others showed almost no activity. It is likely related to CeO_2 hydrogen spillover and metal-support interaction (MSI) as previously reported.[3] To further increase selectivity and suppress methane formation, Ru-based bimetallic catalysts supported on CeO_2 with metals like W, Re, and Ni, will be explored to enhance hydrogen spillover.



PE (Mw ~4000) hydrogenolysis under 20 bar H_2.

Catalyst	Product Composition	Particle Size (nm)	Agglomerate size (nm)
Ru/Al_2O_3	Solid	11.2 ± 4.0	~20–40
Ru/TiO_2-rutile	Solid	5.7 ± 1.3	-
Ru/SiO_2	>C25 Wax	11.8 ± 5.15	~30–90
Ru/CeO_2	C9-C16	21.7 ± 7.3	~40–50
Ru/ZrO_2	Solid	37.7 ± 14.6	~80–410
Ru/C	C9-C16	-	-

Liquid product distribution of PE (Mw ~4000) hydrogenolysis using Ru/C.

Fig. 1. Scheme and results of PE (Mw ~4000) hydrogenolysis using Ru-based catalysts.

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EES - D4 - O10

Establishing structure-acidity-performance relationships in zeolite catalyzed lignin pyrolysis for aromatics production

D. Sajwan[1], L. Dorazio[2], A.N. Parvulescu[3], N. Bottke[3], M. Monai[1], B.M. Weckhuysen[1,*°]
[1]Utrecht University, NL; [2]BASF Corporation, USA; [3]BASF SE, DE

Lignin constitutes up to 35 % of biomass, yet only a small fraction is currently valorized to high-value chemicals at an industrial scale.[1] Catalytic pyrolysis over solid acids, particularly zeolites, offers significant potential for producing aromatics-rich bio-oil from lignin.[2] However, the selectivity towards aromatics remains low, primarily due to the complex structure of lignin.[3] Although framework topology and acidity are well studied to govern hydrocarbon pyrolysis performance, their influence on lignin pyrolysis remains poorly understood.[4] Herein, three zeolite topologies (i.e., H-Y, H-ZSM-5, and H-Beta) with varying acidity profiles were investigated for lignin pyrolysis in a semi-batch reactor. Substantial differences in bio-oil yield and product distribution were observed, unraveling the critical role of zeolite topology (Fig. 1A). The highest aromatics yield (126-160 mg/g_{lignin}) was observed for the H-ZSM-5 family, followed by H-Beta (44-68 mg/g_{lignin}) and H-Y (13-34 mg/g_{lignin}) (Fig. 1B). Comparative analysis demonstrated that framework topology exerts a more dominant influence on aromatics production than bulk or external acidity. Aromatics production for the best-performing H-ZSM-5 with a Si:Al ratio of 23 increased with decreasing carrier gas flow and increasing catalyst:feed ratio. Furthermore, this catalyst achieved consistent aromatics yield (148-185 mg/g_{lignin}) with different lignin feedstocks, eliminating the challenge of feed heterogeneity (Fig. 1C). Thermogravimetric analysis (TGA) revealed that the temperature of maximum weight loss (T_{max}) shifts to higher values than thermal pyrolysis regardless of the catalyst used, indicating delayed lignin decomposition due to additional stabilizing zeolite-phenolic interactions (Fig. 1D). These results suggest that the variations in product distributions were attributed to secondary deoxygenation reactions rather than primary depolymerization, leading to enhanced aromatics formation in H-ZSM-5 due to the stronger pore confinement effect experienced by depolymerized fragments (Fig. 1E). Overall, this work presents a detailed experimental assessment of framework topology dependent deoxygenated aromatics production in zeolite catalyzed lignin pyrolysis.

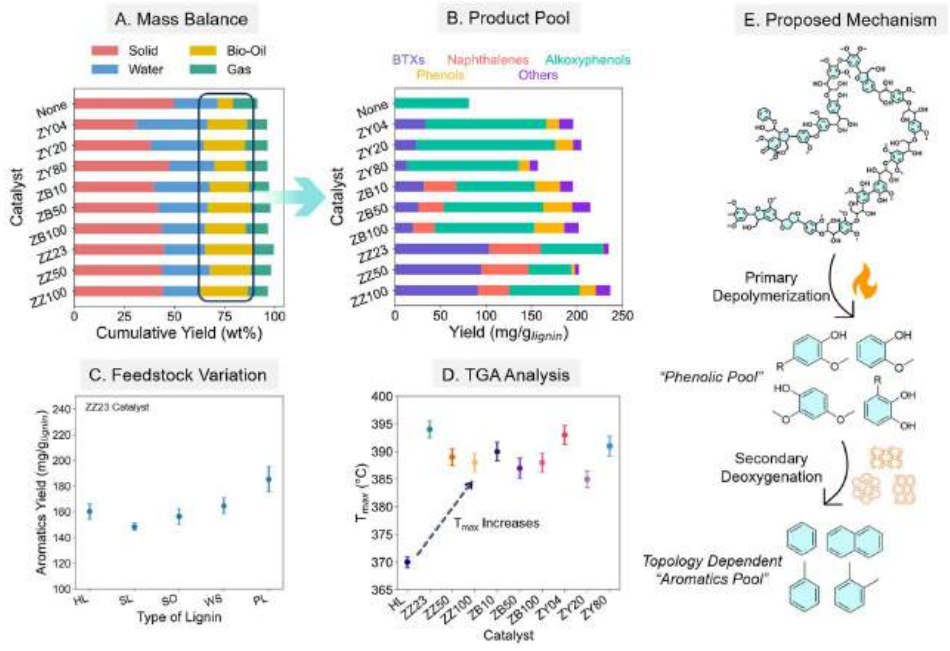

Fig. 1. A. Mass balance plot for thermal pyrolysis and catalytic pyrolysis showing increased bio-oil yield in catalytic pyrolysis, B. Product distribution in bio-oil for different catalytic reactions, C. Aromatics yield (mg/g_{lignin}) for different types of lignin with the ZZ23 catalyst to test the effect of feed heterogeneity, D. Differences in T_{max} observed from TGA for thermal and catalytic pyrolysis reactions, E. Proposed reaction mechanism of initial lignin depolymerization to phenolics pool, which is independent of the zeolite used, followed by a zeolite topology-dependent deoxygenation to yield aromatics. Reaction conditions: Zeolite:Lignin=1:1 wt% (2 g each), 400 °C, 50 ml/min N_2 flow. Abbreviations: Zeolite Y - ZY, Zeolite Beta - ZB, Zeolite ZSM-5 - ZZ, Number = Silicon to Aluminum Ratio (SAR), HL - Hardwood Lignin, SL - Softwood Lignin, SO - Spruce Organosolv Lignin, WS - Wheat Straw Lignin, PL - Poplar Lignin. The yield was analyzed by 2-D GC x GC-MS-FID instrument.

B.M.W. thanks BASF and the Advanced Research Center Chemical Building Blocks Consortium (ARC CBBC) for funding this research. The authors acknowledge Prof. Eelco Vogt, Dr. Florian Meirer, Dr. Sebastian Rejman, and Jochem van de Minkelis for scientific discussions as well as Oscar Kerkenaar (UU) and Joris Janssens (UU) for technical assistance.

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EES - D4 - F02

A systematic computational screening for discovery of low-cost, sustainable thermochemical heat storage materials

Mohammad Monir[1], Zhaochun Liu[1], Veerapandian Ponnuchamy[1], Aleksandr Shkatulov[2], Kingsley Oulah[1], Ionut Tranca[1], Frederik Tielens[1*]
[1]Vrije Universiteit Brussel (VUB), BE; [2]Iberian Energy Storage Research (CIIAE), ES

Thermochemical heat storage (TCHS) offers high energy density and long-term storage capability, making it an attractive solution for renewable energy integration and industrial waste heat recovery, as shown in figure 1[1].

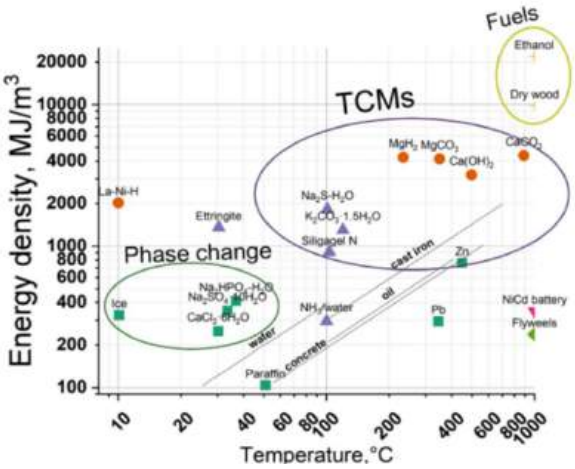

Fig. 1. Comparison of energy storage technologies. “TCMs” stands for thermochemical materials [1].

However, many existing TCHS materials suffer from high cost, reliance on critical or toxic elements, and limited sustainability [2,3]. In this work, we present a systematic computational screening methodology to identify novel, sustainable TCHS materials from large crystallographic databases. More than 600,000 entries from the Crystallographic Open Database, Materials Project, NOMAD, Mindat, ICSD, and RRUFF were screened using a multi-stage Python-based workflow. The selection criteria focused on (i) carbonate–hydroxide (CO_3–OH) or carbonate–hydride (CO_3–H) bonding motifs, (ii) structural verification of bonding environments via CIF analysis, (iii) exclusion of toxic elements and critical minerals, and (iv) assessment of synthesizability. The screening yielded 48 promising candidate materials composed exclusively of earth-abundant elements (Ca, Mg, Na, K, C, O, H). These candidates exhibit decomposition temperatures of 80-175°C and energy storage densities of 0.93 to 4.08 GJ/m^3, competitive with conventional materials while offering significant advantages in cost, sustainability, and safety. Over 60% of identified candidates have documented synthesis routes, indicating strong experimental feasibility. Overall, this work demonstrates an efficient computational approach for discovering sustainable energy materials and identifies a previously underexplored class of thermochemical storage compounds suitable for medium-temperature industrial waste heat recovery applications.

This work is conducted within the framework of the 4Tunates project (https://4tunates.eu/), a European initiative focused on developing next-generation thermochemical heat storage solutions.

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EES - D4 - F03
Presodiation as a key strategy for stabilizing sodium-ion batteries

Rita Carvalho Veloso[1,2*],Carolina Saraiva[1,2], Gonçalo Leite[2,3], Miguel Duarte[3,4], Adélio Mendes[1,3,4]
[1]Chemical Engineering Dept., Faculty of Engineering University of Porto, PT; [2]Vasco da Gama CoLAB – Energy Storage Associação, PT; [3]LEPABE, Faculty of Engineering University of Porto, PT; [4]ALiCE – Associated Laboratory in Chemical Engineering, Faculty of Engineering University of Porto, PT

Sodium-ion batteries (SIBs) offer a cost-effective and abundant alternative to LIBs, with analogous operating principles. Their main limitation arises from the larger and heavier Na^+ ions, which reduce energy density. Presodiation is a technique used to compensate for irreversible sodium losses during the initial cycles, thereby improving cell lifespan[1]. This is a key strategy for SIBs, which typically have lower energy density, specific capacity and lifecycle compared to lithium-ion batteries. There are several methods for presodiation, however the use of sacrificial salts has demonstrated to be a simple, cost-effective and industrially scalable approach[2]. In this work, sacrificial sodium salts are studied as a simple, scalable and industrially viable presodiation strategy. SIB cathode systems were evaluated in combination with different sacrificial additives and loadings, and their electrochemical performance was assessed in half-coin cells. Electrochemical results demonstrate that both sacrificial salts effectively mitigate irreversible capacity losses and improve cycling stability. Comparative analysis highlights the critical role of cathode structure and additive chemistry in optimizing presodiation efficiency.
Overall, this study provides practical insights when designing presodiation strategies tailored to different cathode chemistries, reinforcing the potential of sacrificial salt-based approaches to accelerate the development of high-performance SIBs.

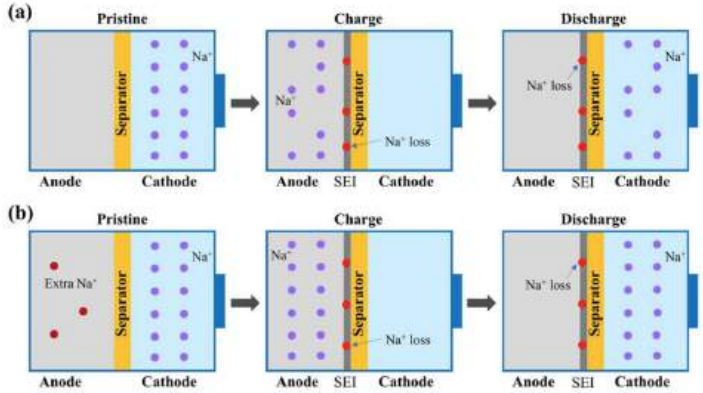

Fig. 1. Schematic representation of a SIBs a) without and b) with presodiation[3].

This work was supported through the PRR project 01/C05-i02/2022.P269 – “Missão Interface”, funded by the Recovery and Resilience Plan (Plano de Recuperação e Resiliência – PRR) of the Portuguese Republic, under the NextGenerationEU framework.

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EES - D4 - F04
Polyhalite Stability in Salt Solutions at 25 °C : A Long-Term Investigation

Lena Bonitz[1], Daniela Freyer[1], Gero Frisch[1]
[1]TU Bergakademie Freiberg, DE

Polyhalite, $K_2SO_4 \cdot MgSO_4 \cdot 2CaSO_4 \cdot 2H_2O$, is found in salt rocks, which are being considered as radioactive waste repositories. Understanding the cocentrations of species that may develop upon contact with the minerals of surrounding salt rocks is critical for assessing radionuclide interactions in scenarios involving solution inflow.
This study investigates the stability field of polyhalite, addressing discrepancies in literature[3] (marked pink) and models (HMW[1], marked blue; THEREDA[2], marked red; Figure 1). The two models currently in use do not agree at a temperature of 25 °C.

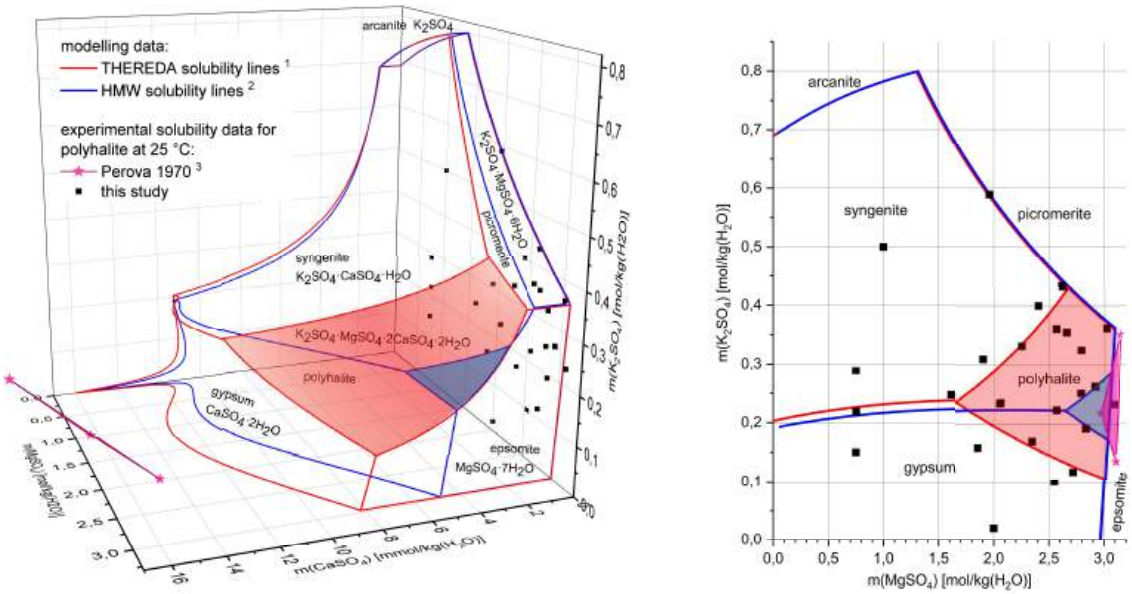

Fig. 1. Polyhalite stability fields in the system K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-} - H_2O at 25 °C according to THEREDA and HMW (left) and a projection onto the K_2SO_4-$MgSO_4$ surface (right) with the the initial solution concentrations (black points) from this investigation.

Solution-solid mixtures were prepared for long-term equilibration, with initial solution concentrations ($CaSO_4$ free) corresponding to the black points in Figure 1. Various calcium sulfate containing solids: hemihydrate, $CaSO_4 \cdot 0.5H_2O$, gypsum, $CaSO_4 \cdot 2H_2O$, polyhalite, $K_2SO_4 \cdot MgSO_4 \cdot 2CaSO_4 \cdot 2H_2O$ and syngenite, $K_2SO_4 \cdot CaSO_4 \cdot H_2O$, were added to these 23 solutions resulting in 88 solution-solid mixtures. Changes in the solid phase composition were analyzed using Raman spectroscopy. Raman analyses demonstrated transformations of the initial phases syngenite, gypsum, and hemihydrate. For all three syngenite formed at higher K_2SO_4 concentrations, while gypsum dominated at lower concentrations. After 1.5 years small polyhalite crystals began to form in most of the solutions and first changes have been detected in the samples with polyhalite as initial phase.
The next important step is to analyse the liquid phase. Due to very low $CaSO_4$ concentration alongside high $MgSO_4$ concentrations a practical method has been found. Since different solid phases are still present at identical solution compositions, equilibrium has not yet been reached, but ongoing efforts aim to determine the polyhalite stability field for the first time at 25°C in this quaternary system.

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EES - D4 - F05
Light-matter interactions in carbon nitride-based photocatalysis

Maria J. Sampaio[1], Joana C. Lopes[1], Cláudia G. Silva[1], Joaquim L. Faria[1*]
[1]LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, PT

A detailed understanding of light-matter interactions is essential for advancing photocatalytic routes towards sustainable chemical processes. Within this context, heterogeneous photocatalysis has emerged as a critical platform for energy conversion, environmental remediation, and selective chemical transformations. The research activities of our group focus on the fundamental design, modification, and application of semiconductor photocatalysts, with particular emphasis on graphitic carbon nitride-based materials.
Photocatalytic systems are investigated across a range of chemically relevant processes, including water and wastewater treatment, solar-driven hydrogen generation, and the transformation of biomass-derived substrates into value-added chemicals[1,2,3,4]. Across these applications, graphitic carbon nitride is a common material framework due to its visible-light activity, chemical robustness, and structural adaptability.
Carbon nitride-based catalysts are engineered through controlled structural, compositional, and interfacial modifications, enabling systematic investigation of charge carrier generation, separation, and surface reaction pathways. These strategies allow precise tuning of catalytic performance for targeted photocatalytic applications. Strong emphasis is placed on operation under chemically realistic conditions, facilitating evaluation of scalability and technological implementation.
Photocatalytic behaviour is examined under realistic reaction conditions, including complex water matrices and renewable feedstocks, allowing fundamental material properties to be directly linked to functional performance beyond idealised model systems. The integration of materials chemistry with photocatalytic mechanisms provides a coherent framework for the fundamental understanding and rational development of photocatalysts for environmental and energy-related applications.

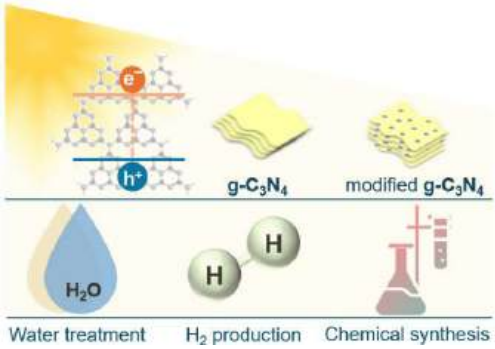

Fig. 1. Illustration of visible-light photocatalytic applications using carbon nitride-based catalysts.

Acknowledgements: This work was financially supported by Fundação para a Ciência e a Tecnologia, I.P./MECI through national funds: LSRE-LCM, UID/50020/2025 (https://doi.org/10.54499/UID/50020/2025); and ALiCE, LA/P/0045/2020 (https://doi.org/10.54499/LA/P/0045/2020). We would also like to thank the scientific collaboration under projects: 2022.04682.PTDC (SuN2Fuel) and COMPETE2030-FEDER-00778800 funded by ERDF through COMPETE2030 and by national funds through FCT - Fundação para a Ciência e a Tecnologia (FCT). Maria J. Sampaio thanks FCT for funding through the Scientific Employment Stimulus - Institutional Call (DOI:10.54499/CEECINST/00010/2021/CP1770/CT0011).

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EES - D4 - F06

Enhancing faradaic efficiency in electrochemical CO_2 reduction via fermentation-derived acid intermediates

Richard Buchinger[1], Yashraj Kumar Singh[1], Markus Valtiner[1], Christian M. Pichler[1]
[1]Institute of Applied Physics, Vienna University of Technology, AT

Defossilization of the chemical industry is one of the major challenges of our modern society. Carbon dioxide (CO_2) should not only be considered a greenhouse gas but also as a valuable resource to produce high-value chemicals. In recent years electrochemical CO_2 reduction (eCO_2R) has attracted significant attention within the scientific community. Considerable effort has been devoted to avoid the energetically unfavorable and kinetically challenging oxygen evolution reaction (OER) at the anode, and several reactions such as glycerol or 5-hydroxyfurfural oxidation to value-added chemicals have been successfully coupled with CO_2 reduction.[1-3] However, the market size of these reaction products remains limited. Ethene, by contrast, is a highly sought-after chemical as it acts as a key chemical intermediate used for the production of polyethylene, alcohols or vinyl chloride.[4]

In a novel approach, eCO_2RR was coupled with the decarboxylation of propionic acid to ethene as a deviation from the classical Kolbe reaction using carbon felt electrodes enabling combined Faradaic Efficiencies for C_{2+} products above 100 %. Notably, the feasibility of utilizing propionic acid-containing microbial fermentation broths was successfully demonstrated. This represents an important step toward sustainable processes, as waste feedstocks (e.g. food waste) can serve as carbon sources for microbial fermentation thereby improving the overall environmental footprint.

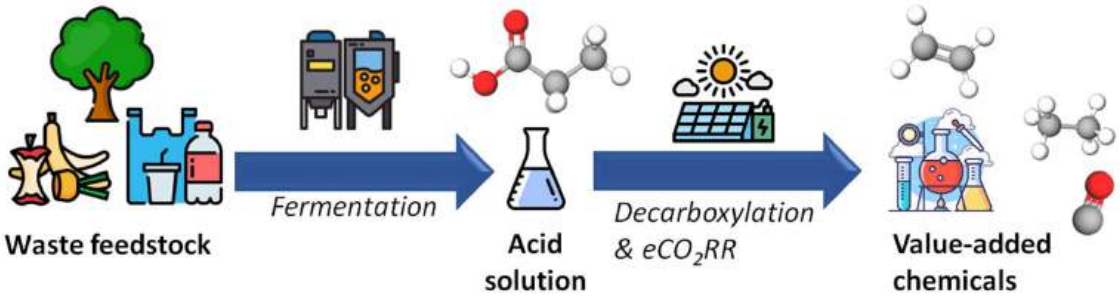

Fig. 1. Scheme of the process from waste feedstocks to value-added chemicals

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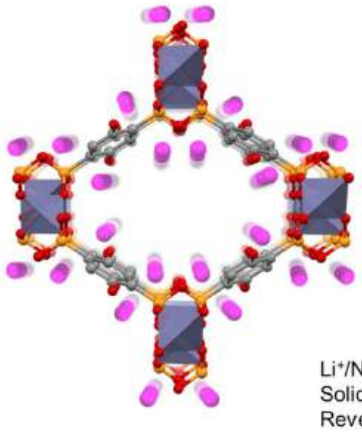
EES - D4 - F10

Bimetallic anionic organic frameworks with solid-state cation conduction for charge storage applications

Augustin Ramackers[1], Alexandru Vlad*[,1]
[1]*Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, BE*

Metal–organic frameworks (MOFs) have recently emerged as an important and challenging class of electrochemical energy storage materials. While previous examples of alkali-containing MOFs are mainly based on carboxylate linkers, new category of materials must be studied to exceed carboxylate limitations. Herein, we present a new phosphonate-based anionic bimetallic organic framework, with the general formula of A_4-Zn-DOBDP (wherein A is Li^+ or Na^+, and $DOBDP^{6-}$ is the 2,5-dioxido-1,4-benzenediphosphate ligand) prepared and characterized for energy storage applications.[1,2] With four alkali cations per formula unit, the A_4-Zn-DOBDP MOF is found to be the first example of non-solvated cation conducting MOF with measured conductivities of 5.4×10^{-8} Scm^{-1} and 3.4×10^{-8} Scm^{-1} for Li_4- and Na_4- phases, indicating phase and composition effects of Li+ and Na+ shuttling through the channels. Three orders of magnitude increase in ionic conductivity is further attained upon solvation with propylene carbonate, placing this system among the best MOF ionic conductors at room temperature. As positive electrode material, Li_4-Zn-DOBDP delivers a specific capacity of 140 $mAhg^{-1}$ at a high average discharge potential of 3.2 V (vs. Li^+/Li) with 90 % of capacity retention over 100 cycles. The significance of this research extends from the development of a new family of electroactive phosphonate-based MOFs with inherent ionic conductivity and reversible cation storage, to providing elementary insights into the development of highly sought yet still evasive MOFs with mixed-ion and electron conduction for energy storage applications.



Acknowledgements: The major core of the work was funded through FWO and F.R.S.-FNRS under the Excellence of Science program (EOS 40007515).Partial support was received from the European Research Council under the European Union's Horizon 2020 research and innovation program (grant agreement no. 770870, MOOiRE-A.V.).

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EES - D4 - F11

Green and wearable energy storage: Fully sustainable solid-state supercapacitors using pectin derived laser induced graphene and pectin electrolyte systems

Segenet Dagmawi Agegnehu[1], Md Jahidul Islam[1], Aidan J. Quinn[1], Michael Nolan[1], Alessandra Imbrogno[1]*, Daniela Lacopino[1]*°

[1]*Tyndall National Institute, University College Cork, IE*

The growing demand for wearable and disposable electronic devices highlights the need for sustainable energy storage technologies. Developing green energy storage devices that combine environmental sustainability with good electrochemical performance is a significant challenge. Here, we developed sustainable all-solid-state supercapacitors by direct laser writing (DLW) of a renewable pectin precursor to form pectin-derived laser-induced graphene (pLIG) electrodes, coupled with environmentally sustainable electrolyte/separator systems. Laser-induced graphene (LIG) has been widely produced from polyimide and various biomass precursors; however, pectin-based LIG has not been reported to date. We evaluated two sustainable electrolyte configurations: (i) a pectin-based hydrogel electrolyte paired with a cellulose separator, and (ii) a pectin-derived solid electrolyte film that functions simultaneously as an electrolyte and separator. The resulting devices exhibited competitive areal capacitance values of 82 and 43 mF cm $^{-2}$ at a current density of 0.1 mA cm $^{-2}$ for the pectin hydrogel and pectin-derived solid-state electrolyte configurations, respectively, corresponding to areal energy densities of approximately 11.4 and 6.0 μWh cm^{-2}, respectively. The solid-state device demonstrated good cycling stability, retaining 89.4% of its initial capacitance after 10,000 charge-discharge cycles. Moreover, the solid-state supercapacitors exhibited excellent flexibility, with the capacitance remaining stable during bending at 60°, 90°, and 120°. The wearable supercapacitor arrays, assembled by integrating multiple single supercapacitor units, demonstrate the ability to power small electronic devices such as LEDs, a wristwatch, a calculator, and an electronic stopwatch, even under bent conditions. This performance highlights the mechanical robustness and practical applicability of the devices for wearable electronics. Such an approach offers promising opportunities for the development of printable and sustainable energy storage materials and devices with enhanced energy density, scalability, and mechanical flexibility.

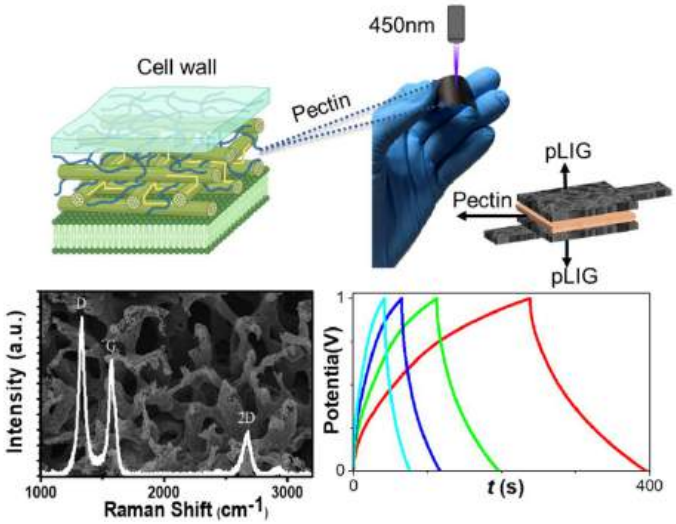

Fig. 1. Schematic of pectin-derived laser-induced graphene (pLIG) fabrication and device concept: a renewable pectin precursor is converted into porous, conductive pLIG by direct laser writing (450 nm) and assembled into an all-solid-state symmetric supercapacitor with a pectin electrolyte/separator. Bottom panels show representative pLIG morphology and Raman spectrum (D, G, and 2D bands) and galvanostatic charge discharge profiles at different current densities.

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Innovative Materials (IM)

IM - D1 - O01

Emergent giant chiroptical response in thin films of a chiral organic dye

Marco Bertuolo[1], Andrea Taddeucci[1,2], Francesco Zinna[1], Gennaro Pescitelli[1], Giuliano Siligardi[2], Lorenzo Di Bari[1], Gianluigi Albano[1,3]

[1]Dipt. di Chimica e Chimica Industriale, Università di Pisa,IT; [2]Diamond Light Source, Ltd., UK; [3]Dipt. di Scienze Chimiche, Università degli Studi di Parma, IT

Investigating optoelectronic applications of thin films of chiral organic π-conjugated materials is an area of active research.[1] In most cases, the differential absorption or emission of circularly polarized (CP) light of these systems is relatively small (dissymmetry factors in the order of $10^{-2}/10^{-3}$),[2] making impossible their practical applications in devices. Although electronic circular dichroism (ECD) and circularly polarized luminescence (CPL) depend on film thickness, values exceeding 500 nm are often required to achieve a sufficiently high degree of circular polarization for use in devices. Unfortunately, such thick structures are not compatible with most devices, as increasing thickness typically diminishes device performance. Therefore, there is a strong interest in developing new chiral organic π-conjugated materials with very strong chiroptical activity (ellipticity > 1 deg) in thin films with a thickness of tens or at most a few hundred nanometers.

In this study, we developed a new chiral indaceno[1,2-*b*:5,6-*b'*]dithiophene bis-thiophenylpropynone (**IDT-TPO**) dye exhibiting unprecedented chiroptical properties in drop-casted and spin-coated thin films (**Figure 1**). While freshly prepared samples are ECD-silent, simple ageing (up to 24 h) induces an extraordinary increase of dichroic response, reaching ellipticity values θ ≈ 18000 mdeg: among the highest reported to date for thin films of chiral organic dyes as neat materials. This amplification is accompanied by an unusual flattening of the main UV-Vis absorption band, resulting in g_{abs} exceeding 0.3. The rationalization of such unconventional properties was accomplished with the support of time-dependent density functional theory calculations and a thorough investigation with spatially resolved chiroptical techniques, including synchrotron radiation Mueller matrix polarimetry imaging (SR-MMP*i*) and circularly polarized microscopy (CPM).

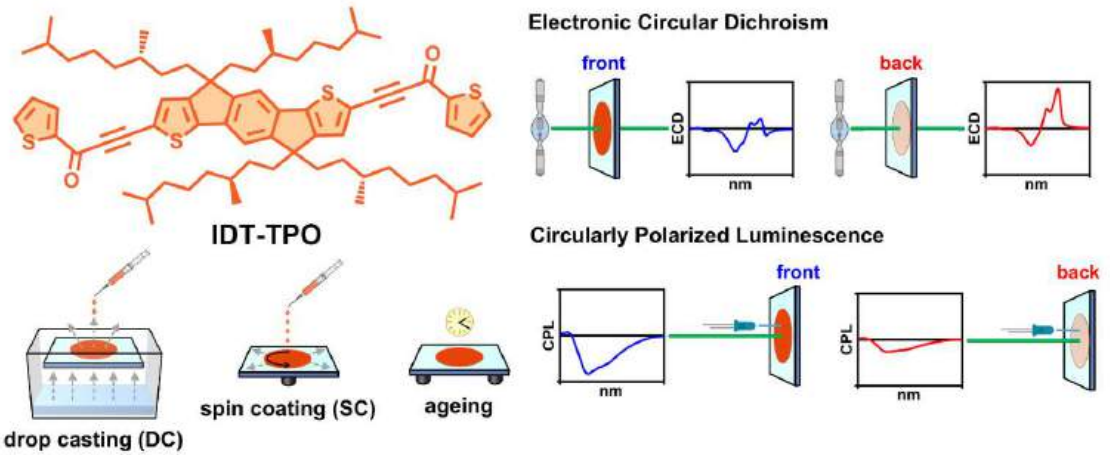

Fig. 1. Chiral **IDT-TPO** dye with giant chiroptical properties in thin films investigated in this work.

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IM - D1 - O02

Porphyrin-based molecular qubits: Spin-polarization mechanisms and surface deposition strategies

Chiara Baldi[1], Prem Prakash Sahu[1], Alberto Privitera[1], Ryan M. Young[2], Federico Totti[1], Michael R. Wasielewski[2], Mathias O. Senge[3], Lorenzo Sorace[1], Stefano Carretta[4], Roberta Sessoli[1]

[1]University of Florence, IT; [2]Northwestern University, IL, USA; [4]Trinity College Dublin, IE; [5]University of Parma & UdR INSTM Parma, IT

Porphyrin-based metal complexes are investigated for Quantum Information Science thanks to their unique optical and electrical properties[1]. Recent research has demonstrated that suitable organic chromophores appended to metalloporphyrins enable optical spin-polarization at room temperature (RT) and photogeneration of multi-level spin states[2,3]. Beyond their photophysical properties, porphyrin-based systems are also suited for integration into solid-state platforms: their flat and thermally stable structures enable ordered surface deposition by thermal sublimation[4].

On this basis, we designed and characterized a new porphyrin-based vanadyl–chromophore dimer (VO-Ph-FP) incorporating a phenyl spacer between the units (Fig.1a). Compared to the prior VO-FP complex[3], DFT calculations revealed significant exchange coupling constant decrease (J_{ex}=–0.12cm^{-1} vs J_{ex}=–0.70cm^{-1}). Transient-absorption spectroscopy experiments at RT were performed by selectively photoexciting the FP unit, revealing an enhanced intersystem crossing time of 126ps and a triplet recombination time of 165μs. The overall slower rates of the photophysics compared VO-FP system[3] is consistent with increased qubit-chromophore separation. Time-resolved EPR experiments in isotropic and aligned media showed emissive spin-polarization evolving into absorptive signals at 85K (Fig.1c). Preliminary simulations point to a polarization mechanism driven by an intermediate exchange regime between VO doublet and FP triplet.

Beyond photophysics, controlled surface deposition is essential for solid-state integration of porphyrin qubits. In a separate study the thermal evaporation of a heterometallic VO–Cu porphyrin dimer (Fig.1b) was investigated, demonstrating that its high thermal stability enables deposition by thermal sublimation. Under ultra-high-vacuum conditions (10^{-11}mbar) sublimation occurs between 350-400°C. XPS experiments confirmed successful deposition, thus excluding thermal degradation[5] and demonstrating the high potential of porphyrin-based qubits.

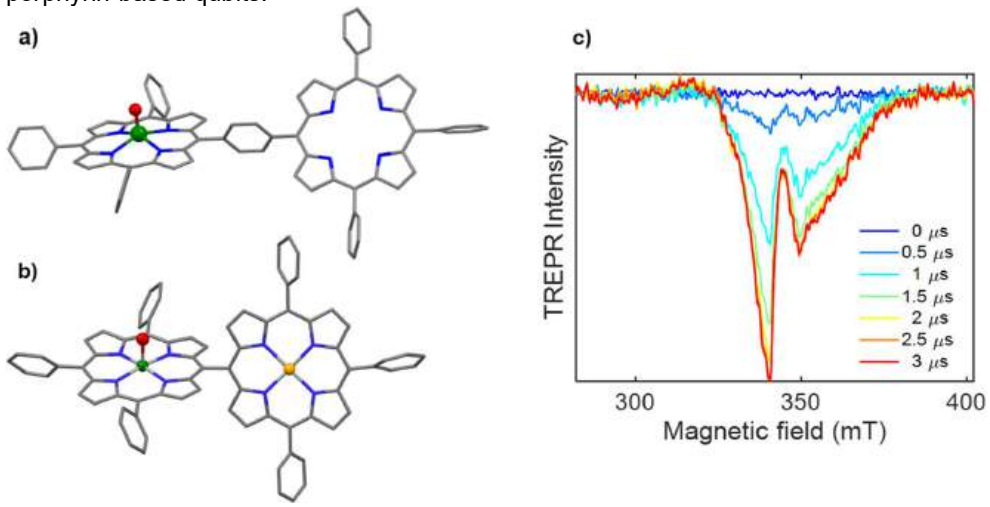

Fig.1. a)VO-Ph-FP dimer, b)VO-Cu dimer: Color code: C=grey, N=blue, V=green, O=red, Cu=orange. c)Isotropic TR-EPR spectrum (85K) at different times.

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IM - D1 - O03

Unveiling diradical control of single-molecule conductance: Beyond the HOMO–LUMO picture

Sergio Moles Quintero[1], Mercedes Alonso[1]
[1]*Vrije Universiteit Brussel, BE*

Advancing molecular electronics requires precise control over charge transport at the single-molecule level, yet this remains challenging because electron transmission in organic frameworks is highly sensitive to subtle changes in electronic structure, conjugation topology, and molecular geometry. In open-shell systems, the presence of unpaired electrons perturbs the π-manifold, enabling resonance structures and spin delocalization patterns that can drastically alter conductance pathways.

Organic diradicaloids provide a promising platform to address these challenges because their electronic structure intrinsically links geometry, aromaticity/quinoidization, and spin distribution. Their partially open-shell character allows fine modulation of π-delocalization patterns. This tunability directly impacts conductance: increasing diradical character weakens central double bonds, enhances torsion, modifies orbital localization, and alters interference conditions within the conducting channel. Moreover, the controlled transition from monoradicals to diradicals in well-defined scaffolds allows systematic exploration of how spin–spin coupling and radical injection reshape molecular transport, providing a unique handle not available in closed-shell systems.

In this work, we exploit the responsiveness of organic diradicaloids to build a structure–property framework for single-molecule conductance that transcends HOMO–LUMO metrics. By analysing key electronic integrals governing diradical character and spin delocalization and correlating them with transport signatures, we derive predictive rules linking molecular architecture and open-shell electronic structure to charge transport.

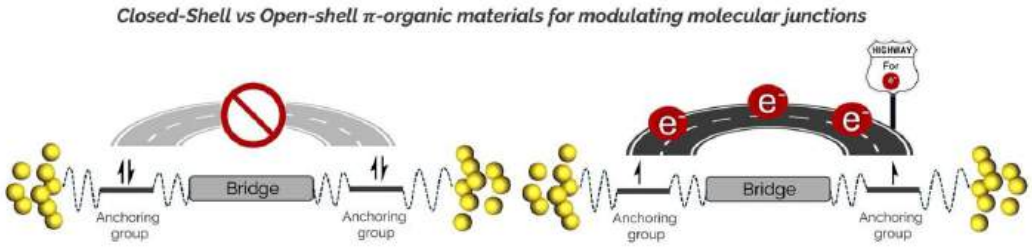

Fig. 1. Schematic comparison between transmission pathways in closed-shell (left) and open-shell (right) π-organic systems in single-molecule junctions.

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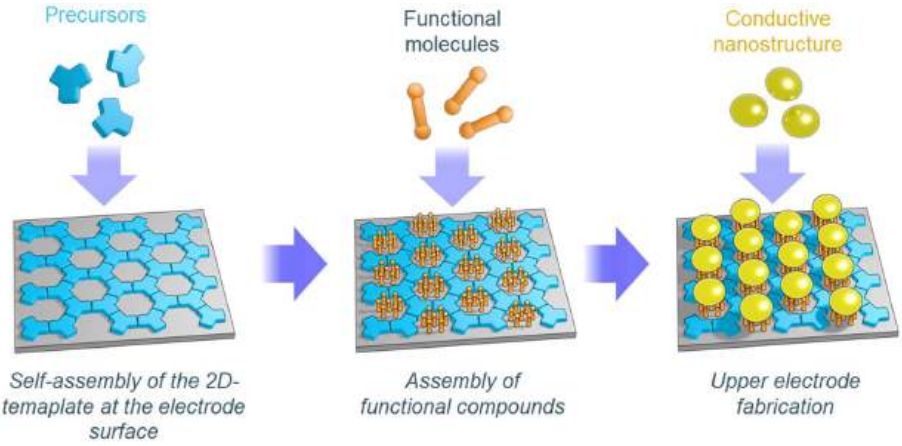
IM - D1 - O04
Molecular templates as platforms for controlled surface fabrication of molecular electronic devices

Enrique Escorihuela,[1,2,3,4] Steven De Feyter,[1] Pilar Cea,[2,3,4]
[1]Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, BE; [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-University of Zaragoza, ES; [3]Physical Chemistry Dept. of the University of Zaragoza, ES; [4]Laboratorio de Microscopias Avanzadas (LMA), University of Zaragoza, ES

The use of molecules as electronic components has garnered significant attention since Aviram and Ratner conceived the idea in 1974. Over the past decades, numerous organic compounds have been studied and demonstrated to function as current rectifiers, resistors, switches, or transistors. However, achieving efficient and reliable electrical contacts to a large number of individual molecules remains one of the key challenges in Molecular Electronics, hindering the fabrication of functional devices.[1]
Herein, we present a compilation of template-based strategies to direct the integration of individual or a limited number of molecules into electronic devices on electrode surfaces. These approaches exploit either the spontaneous self-assembly of organic compounds into molecular networks, such as dehydrobenzoannulene or benzoic acid derivatives, or the use of the Langmuir-Blodgett technique to achieve controlled molecular packing. Therefore, the incorporation of functional electronic molecules by self-assembly or electrografting is governed by the electrode-template interface,[2] in which the molecular patterns either expose discrete regions of the electrode or serve as specific anchoring sites. Finally, the incorporation of the upper electrode, such as metallic nanoparticles, completes the circuit, enabling the measurement of the electrical properties of these systems by conductive scanning probe microscopies, including STM and conductive AFM.
This approach benefits from large-area fabrication techniques by sequentially combining different materials to produce discrete and isolated devices through a relatively straightforward methodology, enabling a high device yield per unit area and allowing modulation of device properties and arrangements based on the shape of the underlying pattern.



Scheme of the fabrication process of isolated molecular devices on the electrode surface.

This work was supported by KU Leuven–Internal Funds (C14/23/090) and the Odón de Buen Postdoctoral Grant from the Government of Aragón.

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IM - D1 - O05

Chemically tuning the intersystem crossing in SWCNTs towards quantum sensing

J. Alejandro de Sousa[1], Ilias Vandevenne[1], Jana Nikolic[1], Tuur Boonen[1], Etienne Goovaerts[1], Sofie Cambré[1]
[1]TSM² group, Physics Dept., University of Antwerp, BE

Chemistry tools are playing a crucial role in designing the quantum properties of functional materials, for instance, by allowing tuning of the excitonic behavior in single-walled carbon nanotubes (SWCNTs). These are emerging as promising one-dimensional platforms for optoelectronics and (bio)sensing applications, where specifically designed chemical interactions and chemical reactions allow one to incorporate a library of new functionalities in their interiors or on their external walls.[1,2]
Controlled sp^3-functionalization of SWCNTs,[3] to generate the so-called quantum defects, has shown to create a potential well that traps excitons, increasing their lifetime and shifting the SWCNT emission to the NIR (by 100-300 meV) with a substantial increase in the PL quantum efficiencies by at least an order of magnitude.[2] However, even though singlet excitons have been extensively studied and exploited for various applications, the behavior of triplet states remained largely unknown.
Triplet states are one of the most promising systems for being implemented as quantum sensors, for instance, NV^- centers have already been exploited for ultrasensitive detection of small magnetic fields, electrical currents, or temperature.[4-6] In a recent work, we decorated SWCNTs with a series of aryl derivatives using diazonium chemistry, and investigated triplet exciton features using optically detected magnetic resonance (ODMR) at cryogenic temperatures (Figure 1a).[7] This technique allows for monitoring the transitions between triplet sublevels in an externally applied magnetic field through the emission from the sample.[8,9] The experimental data (full-field, half-field spectra) and theoretical calculations confirm the tuning of the zero-field splitting from the purely axial symmetry observed for pristine SWCNTs[9] and new dynamics appear with the defect density (Figures 1b-1c). Very recently, we were able to detect new features emerging with increasing temperature, indicating a change in exciton dynamics. Strikingly, we optically addressed the triplet states close to room temperature, opening new avenues towards quantum sensing with SWCNTs.

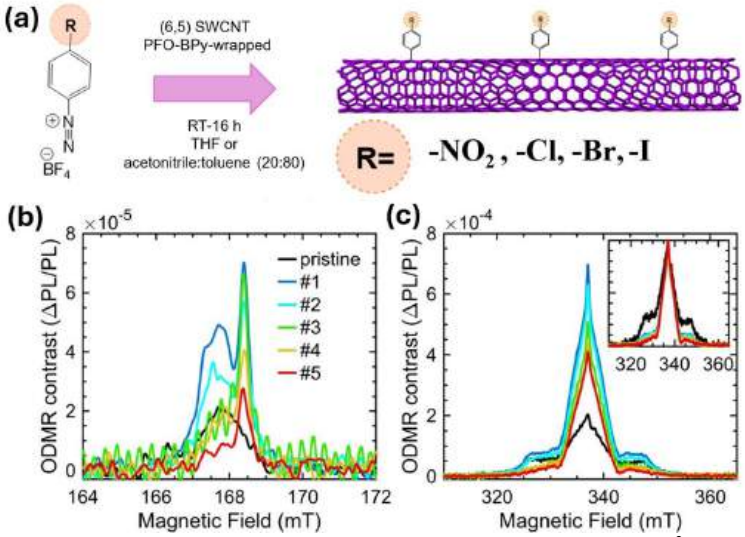

Fig. 1. (a) Chemical modification of polymer-wrapped (6,5) SWCNT with sp^3 defects. (b) Half-field and (c) full-field ODMR spectra of SWCNT-NO_2 samples with different defect densities. All ODMR spectra were acquired in frozen toluene dispersions at T=2.5 K, with laser excitation at 561 nm, a laser power of P=50 mW, a modulation frequency of 374 Hz and by passing the emission through a 1050 nm long-pass filter.[7]

[1]C. Allard et al, *Chem. Soc. Rev.*, **2024**, 53, 8457.
[2]J. Zaumseil et al., *Adv. Opt. Mater.* **2022**, 10, 2101576.
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[9]I. Sudakov et al., *ACS Nano* **2023**, 17, 2190.

IM - D1 - O06
Novel pressure-driven halide substituted spin crossover complexes

Garoé Medina-Aguilar[1], Adrián Sanchis-Perucho[1], María del Carmen Giménez-López[1]
[1]Centro singular de investigación en Química Biolóxica e Materiais Moleculares (CiQUS), ES

Spin crossover (SCO) is a well-known phenomenon that occurs to metal ions with $3d^4$-$3d^7$ electrons, among all compounds, those based in Fe^{II} stand out because they exhibit the largest change between their high spin (HS) and low spin (LS) states, being paramagnetic (S=2) and diamagnetic (S=0) respectively[1]. Two novel neutral mononuclear Fe^{II} SCO complexes substituted with halogen atoms that exhibit spin transition, exclusively under hydrostatic pressure. This pressure-exclusive responsiveness is characterized through variable-pressure techniques[2]. Raman spectroscopy, provides evidence of the progressive structural changes that accompanies mechanical compression, revealing that the pressure required to induce the low spin (LS) state at room temperature shows a dependence on the halide substituent, being 2.03 and 2.17 GPa for compound 1 (Cl) and compound 2 (Br) respectively demonstrating the tunability of the pressure-response through the ligand design. Magnetic measurements in agreement with Raman spectroscopy confirms that the spin transition takes place gradually and it is tuneable when pressure is applied. These new compounds prove that the presence of halogen on the pyridine modifies the transition in comparison with the previous studied compound without halogen substitution compound 3 (H).

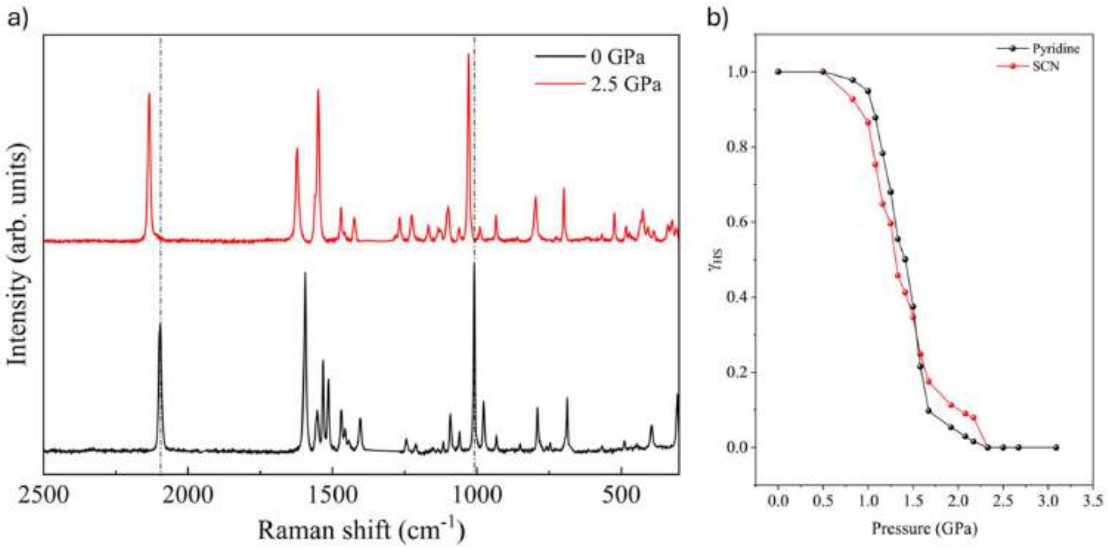

Fig. 1. (a)View of the normalized Raman spectra of compound Br. A gray dashed line serves as a guide to indicate the position of the HS state for the pyridine and the thiocyanate vibrations. (b) γ_{HS} values calculated from the integrated peak areas of the pyridine breathing (Pyridine) and thiocyanate (SCN) Raman modes for compound Cl. The lines serve as a visual aid to connect the points.

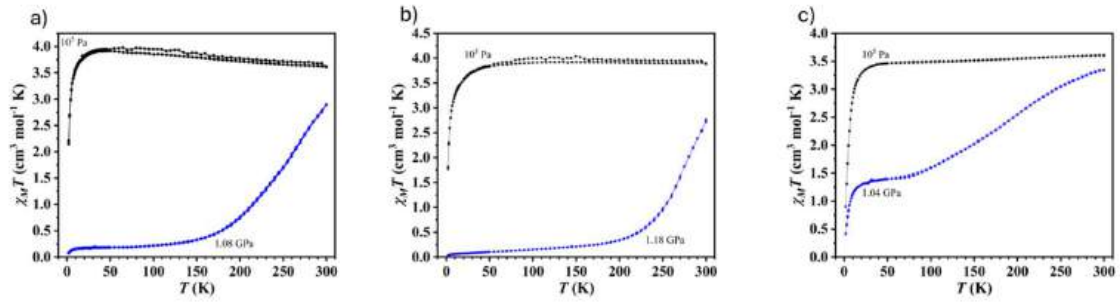

Fig. 2. Temperature dependence of $\chi_M T$ product under a DC applied field of 10000 Oe with a scan rate of 2 K min^{-1} in the temperature range of 2 - 300 K for (a) compound Br. (b) compound Cl. (c) compound H.

Acknowledgements: This work has received financial support from the Ministry of Science of Spain, Agencia Estatal de Investigación (PID2021-127341OB-I00, PID2024-162420OB-I00, CNS2023-145421, and Predoctoral Fellowship FPI for G.M-A.)

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IM - D1 - O07
Triangulating molecular qubits

S. Medina Rivero[1], Z. Ya[2], C. Simms[1], A. de Sousa Rodríguez[1], J. Wu[2], D. Casanova[3], S. Van Doorslaer[1], S. Cambré[1]
[1]TSM[2], University of Antwerp, BE; [2]National University of Singapore, SG; [3]Donostia International Physics Centre (DIPC), ES

In the burgeoning field of Quantum Science and Technology, Molecular Qubits (MQBs) are rapidly gaining momentum due to appealing properties such as the synthetic tunability of their energy levels, and their scalability and precise positioning. A common synthetic strategy to produce MQBs is anchoring two radical moieties through a π-conjugated bridge, with the TTM radical serving as the most widely adopted building block owing to its high emission quantum yield and stability, enabling experimental demonstration of their spin-optical interface, even at room temperature.[1–3] Conversely, non-TTM based diradical MQBs are rare. Organic diradicals reported as promising MQBs with long coherence times[4] often suffer from weak or negligible luminescence, preventing their actual realization as MQBs. Therefore, novel architectures allowing optical readout are highly valuable.[5] In this context, triangulene diradicals are envisaged as promising MQBs,[6] though only recent synthetic advances have yielded stable, luminescent derivatives.[7, 8] Here, we investigate the optical and magnetic properties of an aza-triangulene monoradical and its diradical cation using time-resolved photoluminescence as well as continuous wave and pulsed Electron Paramagnetic Resonance, focusing on HYSCORE experiments to disentangle hyperfine interactions with nuclear spins that govern the relaxation times. We further demonstrate the spin-optical interface for the aza-triangulene diradical using Optically Detected Magnetic Resonance, the technique per excellence for optical readout. Despite the synthetic challenges, we show that MQBs can be successfully encoded in triangulene architectures.

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[2]Kopp, S. M. *et al. J. Am. Chem. Soc.* **2024**, *146*, 27935–27945.
[3]Chowdhury, R. *et al. Nat. Chem.* **2025**, *17*, 1410–1417.
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IM - D1 - O09
Efficient olefin/alkane separation via in-situ cyano-transformed metal–organic frameworks

Chaohui He[1,2], Ben Pilgrim[2]
[1]North University of China, CN, [2]University of Nottingham, UK

Olefin/alkane separation is one of the most critical processes in the global chemical industry and is regarded as one of the "seven chemical separations to change the world".[1] Metal–organic frameworks (MOFs) represent a current research frontier, offering a promising route to address this highly challenging process in an efficient and energy-saving manner. In this work, a series of MOFs were successfully constructed through an in-situ transformation strategy of cyano-containing organic ligands, enabling efficient separation of ethane/ethylene and propylene/propane mixtures. Among these MOFs, the as-prepared NUC-201 underwent site-specific transformation of cyano groups into tetrazolyl groups during the in-situ reaction, creating an ultramicroporous adsorption environment rich in nitrogen-active sites. Single-component adsorption isotherm revealed that NUC-201 exhibits an exceptional ethane uptake of 36.4 cm^3 /g at a low pressure of 0.01 bar, establishing a new record for low-pressure ethane-selective adsorption among reported materials. This performance surpasses benchmark MOFs such as MAF-49,[2] $Fe_2(O_2)$(dobdc),[3] and TYUT-17.[4] In addition, two MOF materials (NUC-202 and NUC-203) were successfully synthesized via an in-situ cyano to amide-imidate conversion, where the original organic ligands were functionalized with methyl and bromo groups, respectively. Size-sieving is recognized as an ideal separation strategy, as it relies on intrinsic differences in molecular dimensions to achieve selective adsorption.[5] By leveraging this strategy, NUC-203 achieved precise pore aperture modulation through bromo group engineering, effectively excluding the larger propane molecules. Consequently, NUC-203 exhibited highly efficient size-sieving separation performance toward propylene/propane mixtures. This work demonstrates the power of in-situ ligand transformation for precise pore environment control, providing fundamental insights into structure–function relationships in MOFs for challenging olefin/alkane separations.

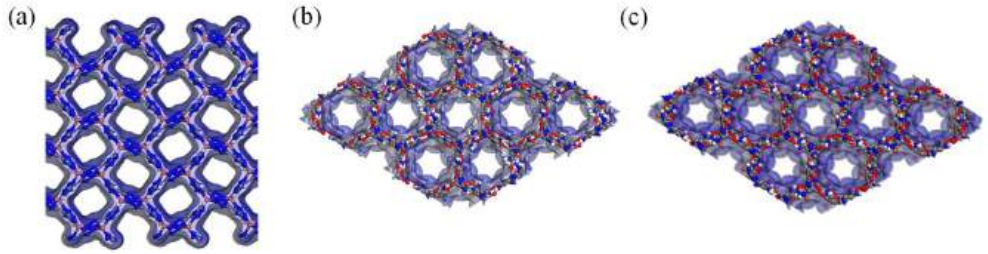

Fig. 1 The crystal structure of (a) NUC-201, (b) NUC-202 and (c) NUC-203.

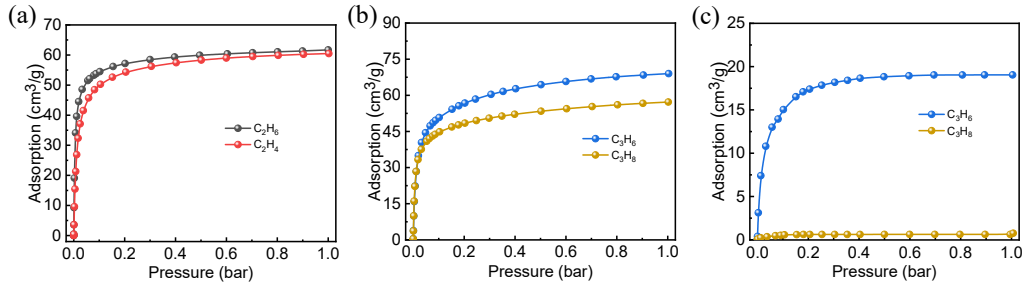

Fig. 2. The single-component adsorption isotherms of (a) NUC-201, (b) NUC-202 and (c) NUC-203 at 298 K.

This work was supported by the National Natural Science Foundation of China (Grant No. 22408353).

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IM - D1 - O10
Macrocycles-based porous organic polymers: Enabling selective molecular separations and more

Alessandro Pedrini[1]
[1]Dept. of Chemistry, Life Sciences and Environmental Sustainability, University of Parma, IT

Macrocycles with preorganized cavities play a prominent role in supramolecular chemistry and materials science, as they are capable of selectively recognizing and capturing specific molecules through the formation of host–guest interactions. To transfer their molecular recognition properties into practical applications, these molecular receptors must be integrated into structured architectures or embedded within polymer matrices capable of preserving the access to their cavities in the solid state.[1] In hierarchically porous materials, for example, the concomitant presence of cavities or pores allows the selective capture and separation of specific molecules from industrially relevant mixtures. This approach was effectively applied to the preparation of a new class of covalent calix[4]arene-based frameworks (CXFs) showing outstanding adsorption properties towards CO_2 and CH_4, while selectively excluding nitrogen (Figure 1a).[2]
More recently, quinoxaline cavitands, which possess the peculiar ability to switch between two well-defined conformations – a compact one, called *vase*, and an extended one named *kite* – were incorporated into polymers of intrinsic microporosity (PIMs).[3] Being characterized by a large dimensional expansion of the molecule driven by the lateral opening of its four walls (Figure 1b), the *vase*-to-*kite* switch was exploited to impart auxetic behavior to PIM-1. Currently, we are investigating the effect of the covalent inclusion of calix[4]arenes with defined conformations into Tröger's base PIMs (PIM-TBs) as a strategy to mitigate their physical aging when used as membranes in gas separation.

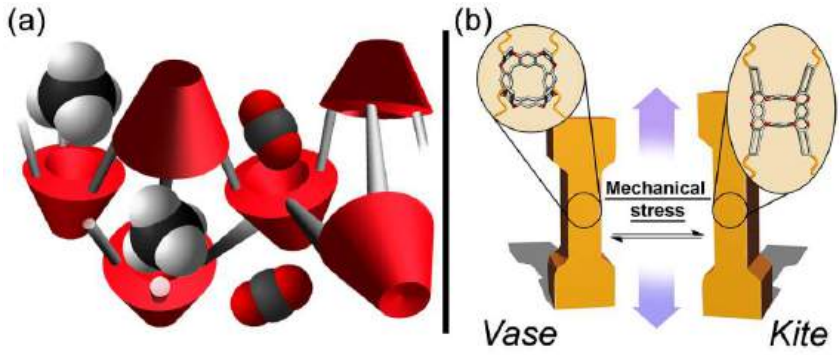

Fig. 1. Molecular recognition with covalent calix[4]arene-based porous organic polymers (a), mechanically induced *vase*-*kite* interconversion in polymer matrices (b).

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IM - D1 - O11

Azo-linked porphyrin-based porous organic polymers for efficient CO_2 capture: An integrated approach

Ivana Biljan[1]
[1]*University of Zagreb Faculty of Science, Dept. of Chemistry, HR*

Emissions of carbon dioxide (CO_2) into the atmosphere remain a primary driver of climate change, posing a serious threat to global environmental stability. Consequently, significant research efforts are focused on the development of advanced porous materials for efficient CO_2 capture, with porous organic polymers (POPs) emerging as promising candidates. Bridging the building units with azo bonds enhances the CO_2 capture capacity and CO_2/N_2 selectivity of POPs. The synergistic combination of azo linkages and porphyrin units, featuring basic pyrrole moieties, further improves the CO_2 uptake of such azo-linked porphyrin-based polymers (APPs).

Building on our recent studies of azo-linked POPs with trigonal connectors,[1–4] we herein extend our research to systems incorporating tetraphenylporphyrin units. We synthesized a series of APPs featuring tetraphenylporphyrin units connected directly or via unsubstituted,[5] functionalized, and sterically hindered linkers. APPs incorporating linkers exhibited significantly higher BET surface areas (167–673 $m^2\ g^{-1}$) than those with directly connected tetraphenylporphyrin units (0.3–23 $m^2\ g^{-1}$), while variations in CO_2 uptakes were less pronounced (15–49 mg g^{-1} at 303 K). Experimental and computational data indicate that azo groups, pyrrole rings, and hydroxyl groups significantly enhance the CO_2 binding affinity of APPs, underscoring a general design principle for CO_2 capture materials.

This work has been fully supported by Croatian Science Foundation under the project IP-2020-02-4467.

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[3]Frey, T., Panić, B., Šutalo, P., Borovina, M., Biljan, I, Kodrin, I. *CrystEngComm* **2023**, *25*, 3870–3884.
[4]Car, Ž., Borovina, M., Panić, B., Biljan, I. *RSC Adv.* **2025**, *15*, 7332–7339.
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IM - D1 - O12

On the importance of balancing the pK_a of the additive in β-ketoenamine COF synthesis

Thijmen A. van Voorthuizen[1], Monique A. van der Veen[2], Louis C.P.M. de Smet[1], Maarten M.J. Smulders[1]
[1]Wageningen University & Research, NL, [2]Delft University of Technology, NL

For quality and safety monitoring and (early) disease detection it is essential to detect specific gas and volatile organic compounds (VOCs). Typically, VOC sensors rely on (porous) affinity coatings to increase their sensitivity and selectivity. The typically high surface areas and chemically tunable pores of covalent organic frameworks (COFs) make them highly suitable for such affinity coatings.
Due to the irreversible tautomerization of imine linkages to their corresponding ketoenamines, β-ketoenamine-linked COFs (Figure 1) are a particularly stable type of COF that display high surface areas, rendering them promising candidates for VOC sensors. In the solvothermal synthesis of such COFs, the use of (acetic) acid is ubiquitous. However, the effect of the added acid on the COF properties (notably their surface area) has never been investigated. Building on an extensive literature overview, we systematically studied the effect of the pK_a of several added acids on COF performance characteristics and extended the investigation by including a series of (organo-)bases with varying pK_a.[1]

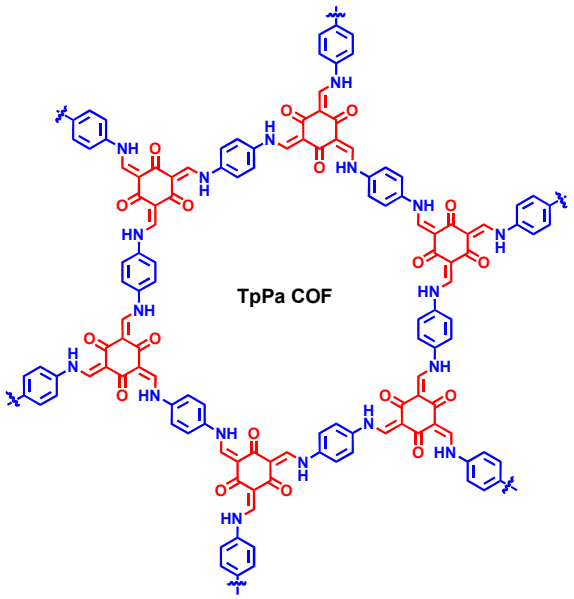


Fig. 1. Chemical structure of the reported β-ketoenamine COF.

Interestingly, the highest BET surface areas, above 1400 $m^2 \cdot g^{-1}$, were found in the alkaline region of the pK_a window, with a maximum near pK_a ~10.8 for triethylamine and *N*,*N*-diisopropylethylamine. Considering the pK_a values related to the three phenolic hydroxyl groups of 2,4,6-triformylphloroglucinol, one of the COF building blocks, these organobases fully deprotonate two of these hydroxyl groups and partly deprotonate the third one, which optimizes the reaction rate of the β-ketoenamine bond formation, explaining the improved COF crystallinity and associated microporosity. The largely overlooked use of organobases in the synthesis of β-ketoenamine-linked COFs thus offers a promising approach to improve the COF performance.

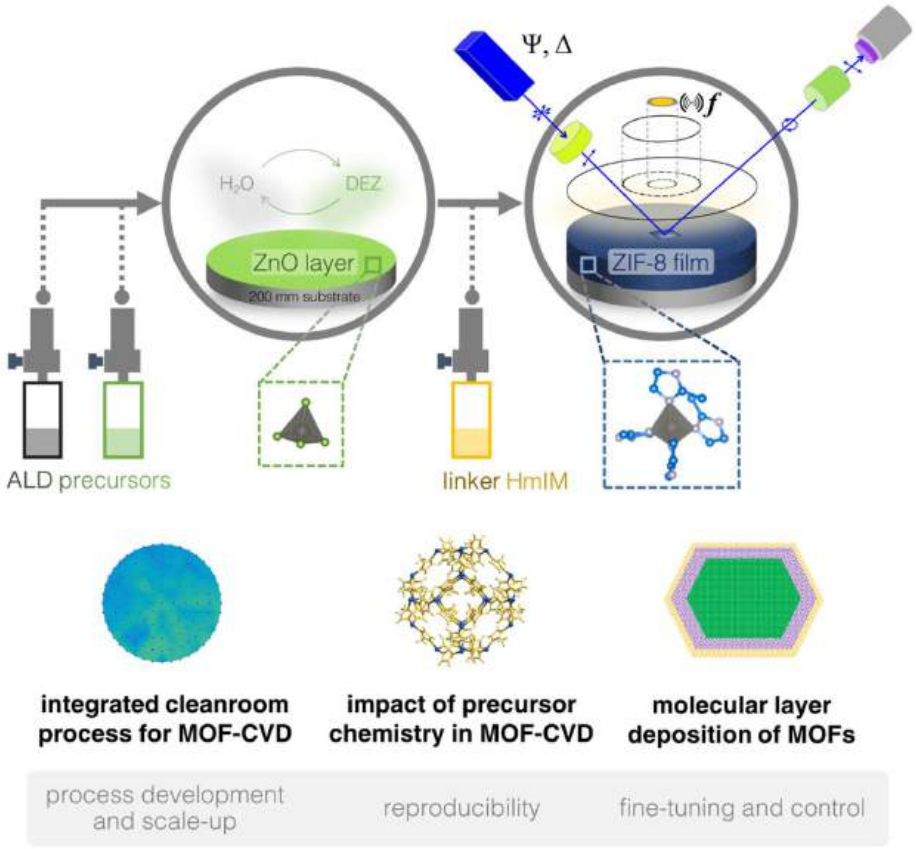
[1]Van Voorthuizen, T. A., Van der Veen, M. A., De Smet, L. C. P. M., Smulders, M. M. J. *Chem. Eur. J.* **2025**, *31*, e202501512.

IM - D1 - O13

Metal-organic frameworks by vapor deposition processes: Polymeric porous materials for integrated applications

Alexander Cruz[1]
[1]*Baker Hughes, BE*

Robust and scalable deposition technologies are key to unlocking the potential of microporous materials in surface chemistry innovation at the nanoscale. The transition towards processing at such dimensions has led to the development of high-performance materials to meet growingly demanding commercial specifications in the energy sector, climate technologies, food science, and cross-disciplines. Metal-organic frameworks (MOFs), a subclass of porous solids comprised of metal-containing nodes connected by polytopic organic linkers, have been gaining attention in the materials science arena. With many interesting attributes such as high specific surface areas, periodicity, and chemical diversity, MOFs have earned their place in the research and development roadmaps of gas storage and transport, catalysis, molecular separations, and, recently, in electronic devices. MOF thin film fabrication techniques compatible with production facilities are a prerequisite to integrating these materials into electronic devices. In this work, the chemical vapor deposition (CVD) and molecular layer deposition (MLD) processes are employed to grow MOF layers entirely from the vapor phase. The spatial uniformity, coating quality, and precise thickness and composition control are key attributes of CVD and MLD, and are a cornerstone to segments requiring cutting-edge innovation in polymer science and materials engineering at large. This presentation tackles the lab-to-fab approach: from mechanistic insights using a range of techniques to process development, optimization, and scale-up. Through the lab-to-fab transition, this work contributes to fully exploiting the colossal potential of MOFs in applications that transcend traditional subject boundaries.



IM - D1 - O14
Nanoporous liquid crystal networks as metallic nanoparticle templates

Alejandro Martinez-Bueno[1,2], Daniele Martella[1,2], Camilla Parmeggiani[1,2]
[1]Dept. of Chemistry "Ugo Schiff", University of Florence, Sesto Fiorentino, IT; [2]European Laboratory for Non-Linear Spectroscopy (LENS), University of Florence, Sesto Fiorentino, IT

Porous polymeric materials have attracted increasing attention due to their permanent porosity, low density, and structural versatility, enabling precise control over chemical functionality and transport properties.[1] Beyond conventional isotropic porous networks, nanoporous liquid crystal polymeric networks have emerged as a particularly attractive subclass, as their porosity and anisotropy can be programmed through liquid-crystalline self-assembly.[2] To date, nanoporous membranes based on columnar liquid-crystalline systems are predominantly obtained through two main strategies: (i) one-component systems relying on the self-assembly of wedge-shaped promesogenic units bearing an ionic head group and a polymerizable end group, and (ii) two-component systems in which a removable template is associated via hydrogen-bonding interactions with wedge-shaped promesogenic units containing polymerizable functionalities. In contrast, an unexplored approach in this field is the use of intrinsically nanoporous networks derived from supramolecular macrocycles formed through hydrogen-bond-mediated interactions[3] between heterocyclic building blocks.
In this work, we present a new class of nanoporous columnar liquid crystal polymer networks based on nucleobase-derived building blocks capable of forming supramolecular macrocycles through directional hydrogen-bonding interactions. The intrinsic nanoporosity of these materials arises directly from the supramolecular organization of the nucleobase units within the liquid-crystalline phase, eliminating the need for removable templates. Furthermore, the adsorption properties of the resulting nanoporous networks are investigated, together with their ability to host and promote the formation of metallic nanoparticles confined within the nanoscale pores.

This work is part of the TEMPL3D project (GA n. 101208850) founded by the Marie Skłodowska-Curie Actions (MSCA) – Horizon Europe Programe (2021-2027).

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IM - D1 - O15

A brand new biomaterial for sustainable electronics: How bacteria invented MOF-based quantum wires ~500 millions years ago

Filip J.R. Meysman[1], Silvia Hidalgo-Martinez[1], Jeanine Geelhoed[1], Cosimo Tommasi[2], Herre van der Zant[2], Eric Boschker[1]

[1]University of Antwerp, Dept. of Biology, BE; [2]Delft University of Technology, Dept. of Quantum Nanoscience, NL

Metal-Organic Frameworks (MOFs) are crystalline materials made of metal ions/clusters (nodes) linked by organic molecules (ligands) into 1D, 2D, or 3D structures. Their modular design allows enables versatile nanoscale construction, and hence, the synthetic design of MOFS is receiving great interest in material science (e.g. Nobel prize 2025).

Our work demonstrates that we humans were not the first to take advantage of the advantage. A recent discovery demonstrates that bacteria already developed MOF structures ~500 millions years ago[2]. These long, filamentous bacteria (called cable bacteria) live in the seabed and are producing centimeter-long thin fibers that are used for long-range electron transport. The conductivity of these wires (> 100 S cm^{-1}) is a million-fold higher than any known biomaterial[2-4], and on or even better par with the most efficient conductive polymers.

The structure that endows exceptional conductance on this fibers is a bundle of thin nanoribbons that form a one-dimensional nickel organic framework[5]. Through confinement these wires show an elevated form of quantum conduction. In effect, the conductivity of these 1-D nanoribbons considerably exceeds the conductivity of the best performing synthetic MOF materials[5]. As such, biology seems to be capable of synthesis of highly regular, thin MOF nanoribbons with exceptional properties. This novel bio-based MOF material could inspire green synthetic and engineering routes for electronic materials based on metal-Organic Frameworks.

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IM - D1 - O16
Functional $K_{3,3}$ ("Kuratowski") building units in materials chemistry: Past, present, and future

Dirk Volkmer[1]
[1]University of Augsburg, Institute of Physics, Chair of Solid State & Materials Chemisty, DE

The first metal-organic framework (MFU-4, Metal-organic Framework Ulm University) comprising "Kuratowski-type" coordination units was reported in 2009.[1] Its strictly orthogonal geometry has inspired chemists to develop a diverse range of functional materials. Owing to a combination of nano-sized cavities and ultra-narrow pores, MFU-4 features kinetic gas trapping allowing for quantum sieving of light hydrogen isotopologues,[2] or high-capacity/slow-release entrapment of noble gas atoms.[3] Gas-specific uptake rates allowed us to construct the first MOF@SAW surface acoustic wave-based sensor.[4] In contrast to MFU-4, the isoreticular MFU-4l(arge) features framework-anchored metal sites resembling the iconic scorpionate complexes (Fig.1).[5] Cu^{I}-MFU-4l shows reversible chemisorption of O_2, N_2, and H_2 with record-breaking isosteric heats of adsorption of 32–53 kJ mol^{-1}.[6] Biomimetic generation of catalytically active Fe^{IV}═O species in Fe-exchanged MFU-4l has recently been demonstrated by Hou et al.,[7] indicating the huge potential of MFU-4-type metal–organic frameworks as catalytic materials.
Apart from the above mentioned applications, framework materials containing Kuratowski-type building units, such as simple M(II)-triazolate frameworks, often show fascinating physical properties, ranging from cooperative large-hysteresis spin-crossover in $[Fe^{II}(ta)_2]$ to spin-liquid behaviour in $[Mn^{II}(ta)_2]$, to name only a few examples.[8, 9] Research activities in our group have recently turned to photoactive metal complexes and frameworks for which the programmable self-assembly of $K_{3,3}$ units offers an efficient bottom-up approach toward artificial photoantenna systems.

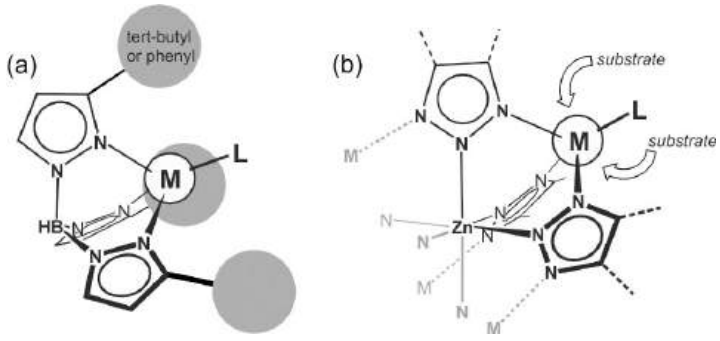

Fig. 1. (a) Scorpionate complex, (b) Secondary building ("Kuratowski-type") unit from MFU-4l comprising open metal sites. (M = transition metal, L = ligand)

[1]Volkmer, D., *Dalton Trans.* **2009**, 6487–6495.
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[3]Volkmer, D., *J.Am.Chem.Soc.* **2018**, 140, 10191–10197.
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IM - D1 - O17

Spectroscopic mapping of tunable metal arrangements in metal-organic polyhedra and frameworks

Paolo Cleto Bruzzese,[1] Qiming Jin,[2] Constanze Neumann[2], Alexander Schnegg[3]
[1]Dept. of Chemistry, University of Turin, IT; [2]Max Planck Institute for Coal Research, DE; [3]Max Planck Institute for Chemical Energy Conversion, DE

Metal-organic polyhedra (MOP) and frameworks (MOFs) are characterized by metal sites embedded in a tridimensional framework which behaves as a solid-state ligand. Although these extended materials can furnish well-defined active sites for the metal centers, their arrangement cannot be tuned in isolation. Changing the relative disposition of a metal site within a crystalline lattice is of paramount importance since it dramatically tailors the material's properties across diverse fields, such as solid-state chemistry,[1] catalysis[2] and quantum sensing.[3]

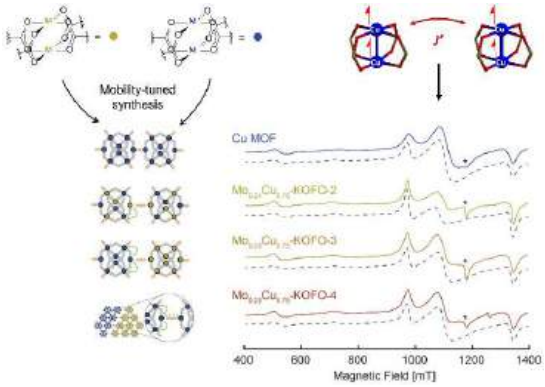

Figure 1: Schematic representation of the metal arrangements synthesized in MOP (left part) together with corresponding EPR spectra (right part). The exchange interaction signal arising from Cu pairs is indicated with the arrow,

Here, a mobility-tuned synthesis approach permits selective synthesis of multiple different “structomers”, which are isostructural and compositionally identical but feature different metal arrangements.[4] High-fidelity access to each targeted metal arrangements is obtained solely through Electron Paramagnetic Resonance (EPR) spectroscopy, using Cu-Cu pairs (*S*=1) as paramagnetic probe. EPR-resolved Cu-Cu exchange interactions (Figure 1) not only discriminate metal distributions within a cage (short-range order) but also across cages (long-range order). Access to both short- and long-range distances supports tuning distance-dependent properties via the extended coordination network.

[1]K. Rossi et al., *Adv. Mater.* **2024**, 36, 2307991.
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[3]P. C. Bruzzese et al., *J. Phys. Chem. Lett.* **2024**, 15 (28), 7161-7167.
[4] Jin Q, Bruzzese P.C. et al. *ChemRxiv*. **2024**

IM - D1 - O18

Bismuth-based metal-organic frameworks as defect-engineered platforms for advanced optical applications

Wafaa Ahmed Mohamed[1], Pascal Van Der Voort[1]

[1]Center for Ordered Materials, Organometallics and Catalysis (COMOC), Dept. of Chemistry, Ghent University, BE

Metal-organic frameworks (MOFs) are highly crystalline materials known for their high porosity, structural tunability, and versatile functionality. Despite their potential, bismuth-based MOFs (Bi-MOFs) remain largely underexplored. In this first-of-its-kind study, we investigate defect chemistry in a novel twofold interpenetrated Bi-MOF (Bi-TATAB) and demonstrate how controlled defect engineering can modulate its structural and optical properties.[1]

Missing-linker defects were introduced in Bi-TATAB without the use of modulators, additives, or post-synthetic treatments. Remarkably, the solvent (DMF) acted simultaneously as a modulator, a co-ligand, and a crystallization medium, revealing a previously unrecognized solvent-mediated mechanism in defect formation. Using a straightforward synthetic approach, defect density was systematically tuned, enabling precise control over porosity, functionality, and photophysical properties (e.g., light absorption, charge transfer, and emission color).

Moderate defect concentrations optimized the MOF's photo-response. Based on this optimization, a rationally selected defect-engineered platform was further doped with Eu^{3+}, Tb^{3+}, Dy^{3+}, Sm^{3+}, and Eu^{3+}/Tb^{3+} via a simple one-pot strategy, yielding highly crystalline, thermally stable mixed-metal MOFs with tunable emission, including white light.[2] The material "$Eu_{0.025}Tb_{0.05}Bi_{0.925}$-TATAB" exhibited outstanding performance as a dual-emitting cryogenic ratiometric thermometer (10-360 K), achieving a maximum relative sensitivity of 8.84% K^{-1} at 60 K, among the highest reported for MOF-based cryogenic sensors to date. The sensor retained robust performance after repeated thermal cycling and three years of storage under ambient conditions.

This work is the first report of defect engineering in Bi-based or interpenetrated MOFs and the first demonstration of Ln/Bi-MOFs for cryogenic thermometry, a rare application for MOFs. Our findings highlight the potential of Bi-MOF platforms for advanced optical applications.

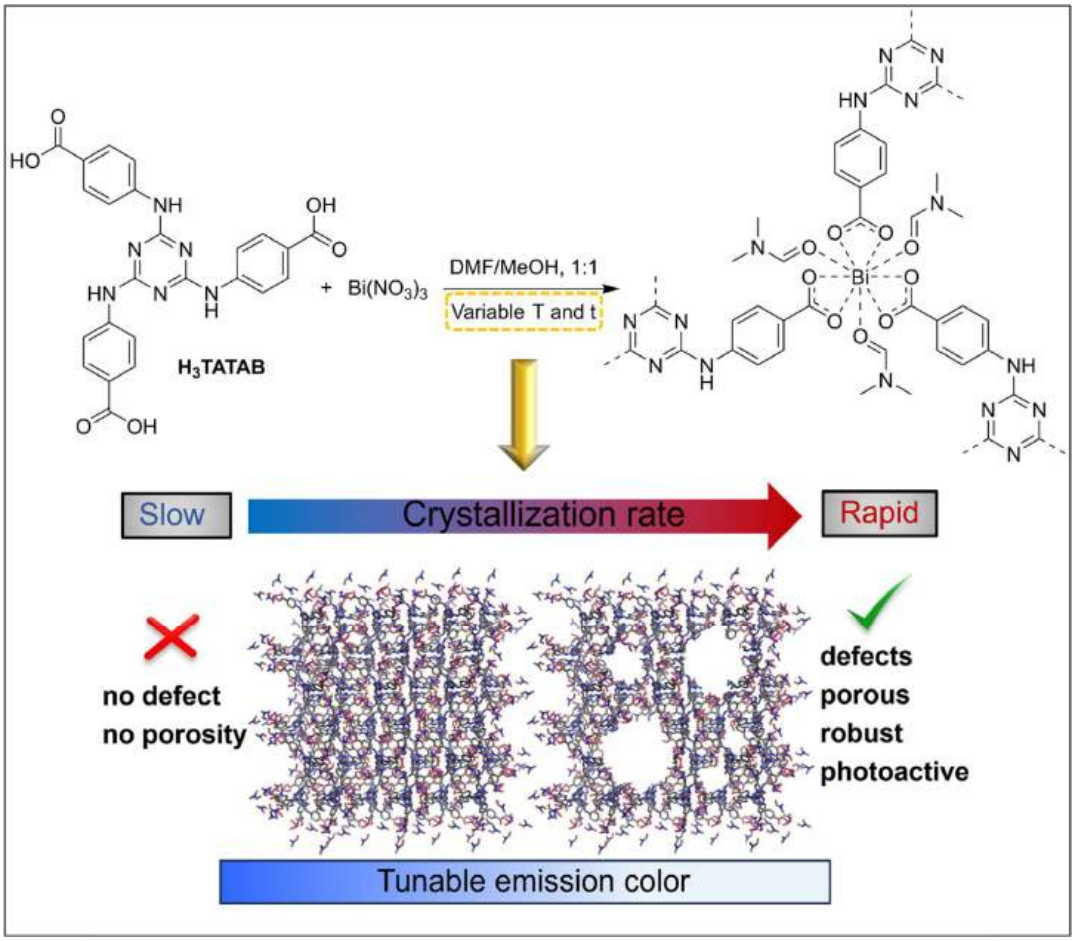

Fig. 1. Synthesis of Bi-TATAB MOF under defect engineering conditions (top), dense Bi-TATAB MOF becomes increasingly defective by a simple change in crystallization rate (as a function of temperature and synthesis time) without structural decay (bottom).

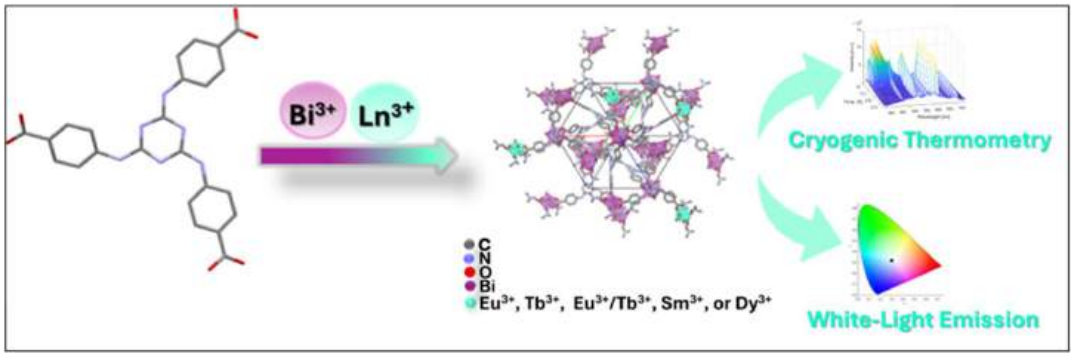

Fig. 2: Schematic illustration of the one-pot synthesis of Ln/Bi-TATAB MOFs and their application as highly sensitive, repeatable, and robust ratiometric temperature sensors and white-light emitters.

[1]Mohamed, W. A., Chakraborty, J., Bourda, L., Lavendomme, R., Liu, C., Morent, R., De Geyter, N., Van Hecke, K., Kaczmarek, A. M., Van Der Voort, P. *J. Am. Chem. Soc.* **2024**, 146, 13113-13125.
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IM - D1 - O19

A strategy to enhance photon upconversion emission in lanthanide metal-organic frameworks

Tapendu Samanta[1], Aleksandra Gerszendorf[1], Szymon J. Zelewski[2], Jan K. Zaręba[3], Min Ying Tsang[1*]

[1]Material Science and Engineering Centre, Łukasiewicz Research Network – PORT Polish Center for Technology Development, PL; [2]Dept. of Experimental Physics, Wrocław University of Science and Technology, PL, [3] Institute of Advanced Materials, Wrocław University of Science and Technology, PL

Lanthanides are known to have specific photoluminescence properties that are attributed to their shielded 4f valence electrons.[1] These unique features allow manipulation of band gaps and thus result in predictable and stable emission bands. One particularly intriguing property is the photon upconversion (UC) process, enabling the conversion of low to high energy wavelengths via sequential two or multi-photon absorption steps. These characteristics make Ln-based materials promising candidates for optical applications. In particular, the UC emission of conventional inorganic phosphors has been utilized in multiple domains, including imaging, optoelectronics, and catalysis.[2] Introduction of Ln into the MOF (LnOFs) system has already been reported for outperforming conventional phosphors.[3] However, the translation of the UC properties from conventional Ln-based phosphors to LnOFs remains largely unexplored.[12–15] Since lanthanide UC efficiency is significantly reduced in materials containing organic ligands, due to competitive nonradiative decay pathways that arise from vibrational coupling mechanisms.[16] Therefore, the proximity of lanthanide centers to organic ligands in MOF structures exacerbates these quenching effects, as the energy transfer efficiency scales with the inverse sixth power of the donor-acceptor separation distance. While conventional strategies rely on short linkers to partially address this, the development of efficient UC-active LnOFs remains challenging. Here we show that engineering multinuclear metal clusters within LnOFs, specifically $\{Y_6(OH)_6(COO)_8\}$ nodes co-doped with Yb^{3+} and Er^{3+}, dramatically enhances UC emission and efficient intracluster energy transfer. This cluster-based strategy circumvents fundamental limitations imposed by organic linkers, establishing a new approach for designing LnOFs with improved UC activity.

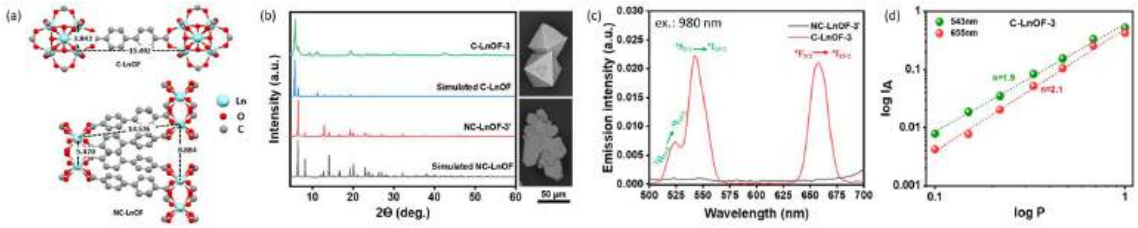

Fig. 1. preliminary data of a) structures of LC-MOF (C-LnOF-3) vs conventional LnOF (NC-LnOF-3'), b) PXRD, c) NIR-to-visible UC emission, Ln = Y0.5/Yb0.3/Er0.2 and b) power dependence.

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IM - D1 - O20

Design and structural characterization of a novel corrole-based covalent organic framework (COF): A strategic approach for metal ion sequestration

Hilal Kalkan[1], Baris Temelli[2]
[1]Gazi University, TR, [2]Hacettepe University, TR

The strategic integration of functional macrocycles into porous architectures is a key frontier in the development of innovative materials for environmental sustainability. Covalent organic frameworks (COFs) have emerged as versatile platforms for such integrations, however, the utilization of corrole macrocycles as structural building blocks within COF architectures remains very limited, with only a few pioneering studies reported in the recent literature[1,2]. Building upon our previous findings where corrole-based systems demonstrated high removal efficiency and excellent reusability in the sequestration of heavy metal ions, this study focuses on the design and precise synthesis of a next-generation corrole-COF material.

We report the synthesis of a novel corrole-based COF via the condensation reaction between an amino-functionalized corrole derivative and [2,2′-bipyridine]-5,5′-dicarbaldehyde (BPyDCA). The structural integrity and long-range order of the framework were rigorously validated through spectroscopic methods and microscopic analyses, supported by theoretical calculations. Preliminary metal-ion adsorption experiments conducted with the synthesized corrole-COF material have yielded promising results, demonstrating high interaction capacity and pronounced selectivity. While the overarching goal of this material design is targeted towards high capacity environmental remediation, this work highlights the successful construction of the COF skeleton and its intrinsic structural advantages. The resulting bifunctional framework establishes a robust foundation for selective metal ion adsorption, expanding the library of innovative porous materials for ecological protection.

Keywords: Corrole-based COFs, Environmental applications, Structural characterization, Innovative Porous materials, Electronic structure

Acknowledgements: This work was supported by the Scientific Research Projects Unit of Gazi University (Project No. FKB-2025-10592).

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IM - D1 - F01

Exploring bioinspired complex coacervates as carriers of cell-loaded liquid-core capsules for biomedical applications

João M. M. Rodrigues[1], Luís. P. G. Monteiro[1], Mariana Carreira[1], Julien Es Sayed[2], Marleen Kamperman[2], João F. Mano[1]
[1]CICECO – Aveiro Institute of Materials, University of Aveiro, PT, [2]Zernike Institute for Advanced Materials, University of Groningen, NL.

In situ thermoresponsive biomaterials, known for their gelation ability in response to physiological temperature, have been widely explored in tissue engineering (TE).[1] However, their combination with complex coacervates remains unexplored. Complex coacervation is characterized as a liquid-liquid phase separation phenomenon that occurs in solutions containing oppositely charged species.[2]
We present an injectable, thermoresponsive complex coacervate based on natural polyelectrolytes designed for TE applications. This complex is formed by combining oppositely charged polyelectrolytes grafted with the thermoresponsive poly(*N*-isopropylacrylamide) (PNIPAAm) polymer. PNIPAAm with amino- and carboxylic acid- terminal groups were successfully synthesized and subsequently grafted onto hyaluronic acid (HA) and chitosan (CHT) (Figure 1) using EDC/NHS coupling chemistry.
Complex coacervation is influenced by i) mixing pH, ii) mixing ratio, and iii) ionic strength. Optimal coacervate was obtained at pH 5.5, using a 1:1 ratio of polyelectrolytes and 100 mM NaCl. Rheological assays revealed shear-thinning behaviour and at 37 °C the hydrophobicity of the system increased. Pre-adherent human adipose-derived stem cells were encapsulated within the coacervate using liquefied core capsules (LC). Loading LC across different volumetric ratios (VR) preserved the shear-thinning profile. The system supported high cell viability and proliferation for up to 7 days, despite the acidic pH required for coacervate assembly.
This engineered biomaterial can incorporate a wide range of cell types and be delivered locally through minimally invasive procedures. Upon activation of its thermoresponsive domains, it conforms to the target site, enabling encapsulated cells to contribute effectively to tissue regeneration (Figure 2).

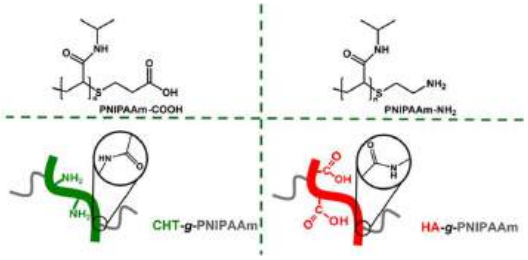

Figure 1 – Polymeric thermoresponsive charged polyelectrolytes.

Figure 2 – Thermoresponsive complex coacervate loaded with liquefied core capsules.

Acknowledgements: This work was developed within the scope of the project CICECO Aveiro Institute of Materials, UID/50011/2025 (DOI 10.54499/UID/50011/2025) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC). Also funded by European Union's Horizon Europe research and innovation programme under the grant agreements BUCCAL-PEP (No. 101091765) and REBORN (ERC-2019-AdG-883370). J.M.M.R. acknowledge FCT for the Assistant Researcher contract (2023.07239.CEECIND/CP2840/CT0004, DOI 10.54499/2023.07239.CEECIND/CP2840/CT0004).

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IM - D1 - F03
Easy access to ε-Fe_2N nanomaterials from Fe nanocrystals

Azadeh EDALAT,[1,2] Catherine AMIENS,[1] Marc RESPAUD,[2] Quyen T. NGUYEN,[3] Phong D. TRAN[3]
[1]Université de Toulouse, CNRS, LCC, FR, [2]Université de Toulouse, CNRS, CEMES, FR, [3]University of Science and Technology of Hanoi, Vietnam Academy of Science and Technology, VN

The nanostructured iron nitride phases, comprising only non-toxic and abundant elements, show potential in a wide range of applications, and are thus of great interest in the context of sustainable development.[1] Especially, the nanostructured ε-Fe_xN phase (x=2-3) can play the role of electrocatalyst (in fuel cells or for hydrogen production), or of anode in Li-ion batteries.[2] However, obtaining morphology and composition (x) controlled nanoparticles of this phase is challenging.[3] Here we show that α-Fe nanoparticles produced by an organometallic approach can be nitridated by a simple exposure to an ammonia flow in mild conditions of temperature (Figure 1), either in the powder form or as thin layers while keeping their initial morphology. Structural and magnetic measurements, combined with chemical analysis, and spectroscopic investigations evidenced the formation of the pure ε-Fe_2N phase, with a preserved nanostructure.[4] We will then show first results on the evaluation of this ε-Fe_2N nanomaterial as electrocatalysts for water splitting and CO_2 reduction. Remarkably, ε-Fe_2N showed promising selectivity toward acetate formation during CO_2 reduction.

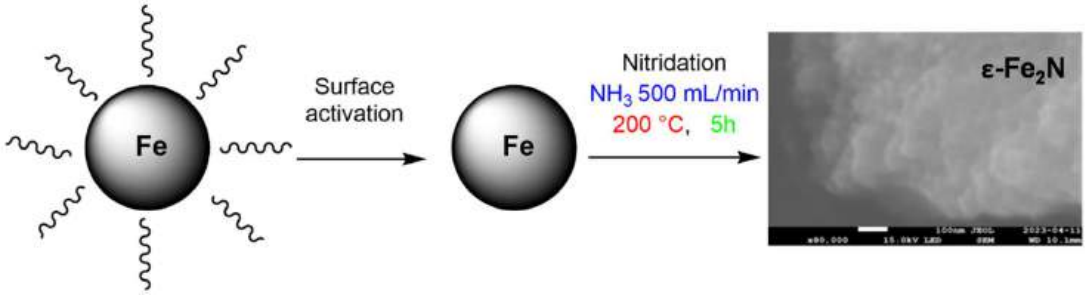

Figure 1 : synthetic procedure towards nanostructured ε-Fe_2N

This work was supported by ANR (projects ANR-19-ASTR-0021-03 and ANR-25-CE50-7591-01), VAST (project THTETN.04/23-24), Région Occitanie and INSA (Project N°00137767 / 22009565).

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IM - D1 - F04
Circularly polarized spin light emitting diodes from chiral two-dimensional superlattices

Mujahid Mustaqeem[1*], Muhammad Ashraf Gondal[1]

[1]*Interdisciplinary Research Center for Hydrogen Technologies & Carbon Management, KFUPM, SA*

Spintronic devices are lined up to drive the next generation of information processing and spin-optoelectronic devices. However, the traditional approaches for controlling spin, charge, and light typically rely on the simultaneous application of electrical and magnetic fields, which complicate the device design and scalability. The discovery of chiral-induced spin selectivity (CISS) provides a compelling alternative by enabling efficient spin polarization without external magnetic fields and opening new avenues for compact and energy-efficient spintronic devices. Despite this promise, initial attempts to integrate CISS into solid-state platforms, such as spin light-emitting diodes (spin-LEDs), have faced significant challenges, including limitations in spin selectivity, modest polarization efficiency, and poor long-term stability, hindering their practical deployment. In this work, we introduce a novel designed strategy based on a chiral molecule-intercalated superlattice to realize efficient and stable circularly polarized spin-LEDs. These chiral superlattice structures are formed by intercalating layered two-dimensional transition metal dichalcogenides (2D-TMDs) with specifically designed chiral molecules, resulting in a highly ordered architecture composed of alternate crystalline atomic layers and embedded chiral molecular layers. This built-in chirality creates an intrinsic spin-filtering environment that strongly enhances spin-dependent charge transport. By employing the chiral two-dimensional superlattice as the active spin-filtering layer, we demonstrate spin-LEDs with an external quantum efficiency (EQE) of ≈18.93% and chirality-dependent circularly polarized electroluminescence (CP-EL) of ±16.5% at room temperature. These performance metrics represent a significant advancement over previous reported CISS-based spin LEDs and highlight the viability of our approach as an alternative to conventional magnetic spin-injection systems. Owing to the wide tunability of transition metal dichalcogenides (2D-TMDs) and the vast structural and chemical diversity of chiral molecules, this platform offers exceptional flexibility. It provides a powerful framework for systematically exploring CISS mechanisms and unlocking their full potential for next-generation spintronic and optoelectronic applications.

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IM - D2 - O01
Emergent giant chiroptical response in thin films of a chiral organic dye

Marco Bertuolo[1], Andrea Taddeucci[1,2], FRsco Zinna[1], Gennaro Pescitelli[1], Giuliano Siligardi[2], Lorenzo Di Bari[1], Gianluigi Albano[1,3]
[1]Dipt. di Chimica e Chimica Industriale, Università di Pisa, IT, [2]Diamond Light Source, Ltd, UK; [3]Dipt. di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università degli Studi di Parma, IT

Investigating optoelectronic applications of thin films of chiral organic π-conjugated materials is an area of active research.[1] In most cases, the differential absorption or emission of circularly polarized (CP) light of these systems is relatively small (dissymmetry factors in the order of $10^{-2}/10^{-3}$),[2] making impossible their practical applications in devices. Although electronic circular dichroism (ECD) and circularly polarized luminescence (CPL) depend on film thickness, values exceeding 500 nm are often required to achieve a sufficiently high degree of circular polarization for use in devices. Unfortunately, such thick structures are not compatible with most devices, as increasing thickness typically diminishes device performance. Therefore, there is a strong interest in developing new chiral organic π-conjugated materials with very strong chiroptical activity (ellipticity > 1 deg) in thin films with a thickness of tens or at most a few hundred nanometers.
In this study, we developed a new chiral indaceno[1,2-*b*:5,6-*b*']dithiophene bis-thiophenylpropynone (**IDT-TPO**) dye exhibiting unprecedented chiroptical properties in drop-casted and spin-coated thin films (**Figure 1**). While freshly prepared samples are ECD-silent, simple ageing (up to 24 h) induces an extraordinary increase of dichroic response, reaching ellipticity values θ ≈ 18000 mdeg: among the highest reported to date for thin films of chiral organic dyes as neat materials. This amplification is accompanied by an unusual flattening of the main UV-Vis absorption band, resulting in g_{abs} exceeding 0.3. The rationalization of such unconventional properties was accomplished with the support of time-dependent density functional theory calculations and a thorough investigation with spatially resolved chiroptical techniques, including synchrotron radiation Mueller matrix polarimetry imaging (SR-MMP*i*) and circularly polarized microscopy (CPM).

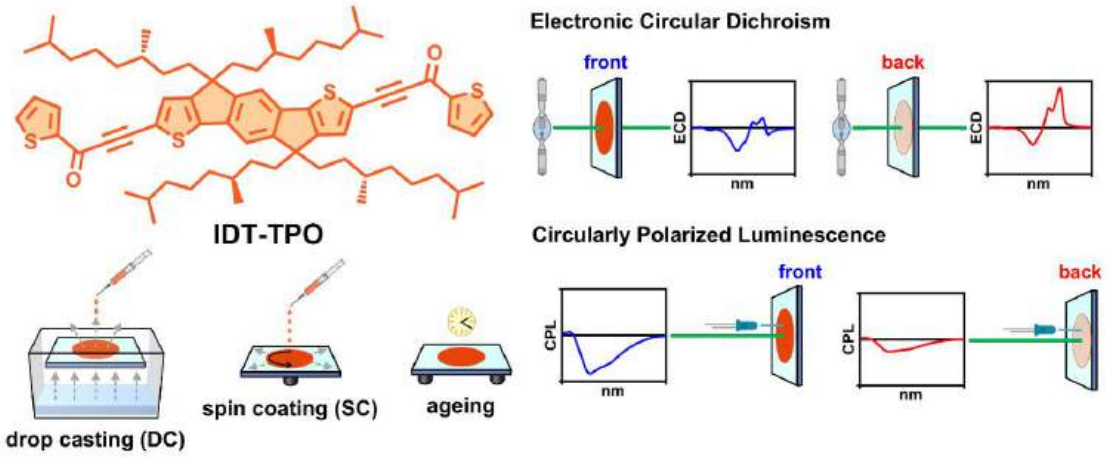

Fig. 1. Chiral **IDT-TPO** dye with giant chiroptical properties in thin films investigated in this work.

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IM - D2 - O02

Fast and programmable electro-active hydrogel micro-actuators fabricated *via* 2PP

Annaël Sort-Montenegro[1], Jason M. Delente[1], Yekaterina Tskhe[1], Ziga Roblek[1], Colm Delaney[1], Larisa Florea[1]
[1]School of Chemistry & AMBER, The SFI Research Centre for Advanced Materials and BioEngineering Research, Trinity College Dublin, IE

Electro-active hydrogels (EAHs) are increasingly investigated for soft actuator applications due to their precise, tuneable response to electrical stimulation.[1] EAHs are crosslinked polyelectrolyte networks that deform *via* electric field–induced osmotic pressure changes, causing asymmetric swelling. However, most EAHs actuators exhibit limited structural complexity and slow response times (minutes to hours), due to volume-dependent hydration processes.[2]

Here, these limitations are addressed by fabricating microscale EAH actuators using two-photon polymerisation (2PP).[3] Three poly(anionic) and poly(cationic) hydrogel photoresists were processed to produce micro-actuators with submicron resolution. This approach enables rapid actuation (<200 ms) and precise control of actuation direction and amplitude through modulation of the applied electric field. Electro-actuation is systematically investigated with respect to actuator charge, geometry, electric field parameters, and electrolyte concentration and pH. Micro-cantilever actuators measuring 80 × 20 × 10 μm³ achieved bending angles up to 44.9 ± 7.8° (n = 591) and actuation times as low as 100 ± 50 ms (n = 22) at 6 V·mm⁻¹.

This study was extended to combine oppositely charged polyelectrolyte hydrogels in a single structure to produce multi-directional actuation under a uniform electric field, while pH-responsive components allowed actuation to be selectively switched on or off. 2PP was also used to create patterned micro-actuators exhibiting both bending and twisting. Additionally, spatial modulation of the electric field using a four-electrode system enabled actuation with increased degrees of freedom, achieving continuous 360° bending of a micro-pillar.

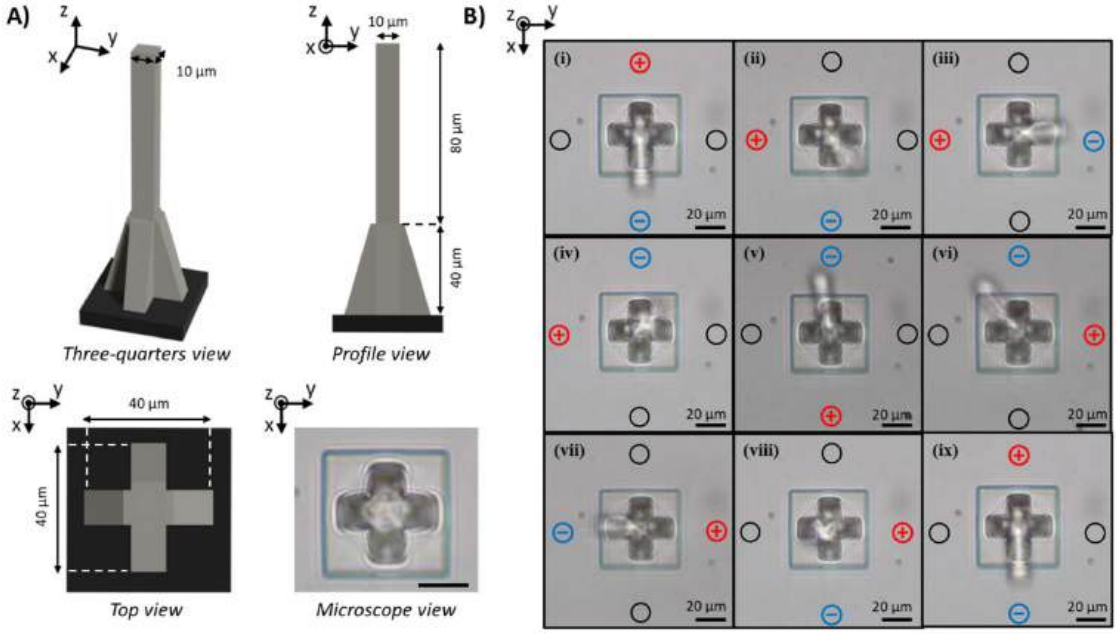

Fig. 1. A) 3D model of the steerable pillar under in different views**. B)** Anticlockwise circular electro-actuation of the pillar in 45° steps from **(i) to (ix)**, circles denote electrode positions and polarities.

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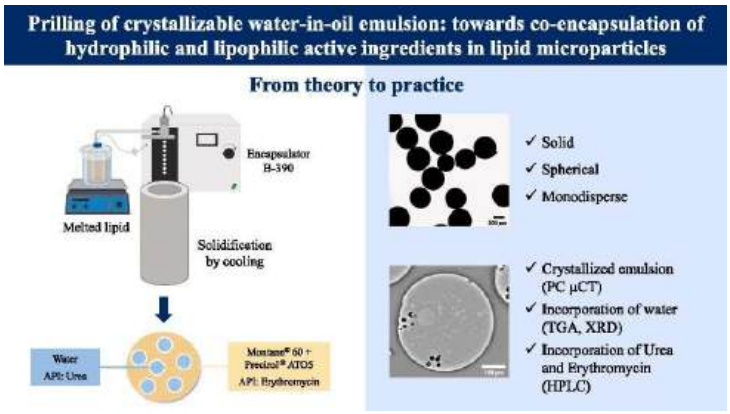
IM - D2 - O03
One-step industrially scalable process for multifunctional hybrid microparticles

Ileana-Alexandra Pavel, Claire Delmas, Julia Toledo Bastos, Vincent Faivre[1]
[1]*Université Paris-Saclay, CNRS, FR*

One of the biggest challenges that both food and pharmaceutical technologies are trying to solve is the low solubility of the bioactive molecules. In the case of functional foods or of the active pharmaceutical ingredients, solubility issues decrease bioavailability and therapeutic efficacy. Moreover, activity of the active molecules can be further drastically reduced *in vivo* due to the transformations during processing and storage, even before further being affected by the passage through the gastrointestinal track.
Lipid-based formulations are a very promising solution to enhance the bioavailability of lipophilic molecules, while encapsulation can enhance the stability of bioactive substances of nutritional or therapeutical interest. By combining these two approaches, co-encapsulation of multiple molecules with different solubilities becomes possible. In the case of industrial-scale applications, an important requirement is that the preparation protocol must be simple and have a low cost. For oral delivery applications, nontoxicity and biocompatibility are also required.



Herein, we present the formulation of multifunctional hybrid microparticles carriers by a one-step industrial scalable process: the prilling technique. Prilling by ultrasonic jet break-up is an efficient process to produce microparticles that are homogeneous in size and perfectly spherical, displaying high encapsulation drug efficiency, controlled drug delivery. This was demonstrated by the incorporation of two model drugs, Erythromycin-hydrophobic molecule into the molten lipids (Compritol 888) and Urea - a hydrophilic molecule into an aqueous compartment[1]. Thus, the two molecules were co-encapsulated into solid microparticles. To increase the bioavailability and to decrease the possible defects generated by the presence of water, silica materials are proposed. These are biocompatible, biodegradable, generally regarded as safe (GRAS), resistant to microbial attack and exhibiting good mechanical strength and thermal stability[2]. The incorporation of silica nanoparticles leads to the production of hybrid lipid–silica microparticles via the prilling technique, resulting in particles with sphericity, and mechanical strength.

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IM - D2 - O04

Size-dependent induction heating properties of octahedron-shaped Fe_3O_4 nanoparticles near the multi-domain limit for (de)bonding on demand applications

Jordi Volders[1,2], Ryan Van Zandvoort[1,2], Iulian Dugulan[3], Bonny Kuipers[4], Ben Erné[4], Marcel Verheijen[5,6], Daniel Mann[1,2,6], Pascal Buskens[1,2,6]

[1]NL Organisation for Applied Scientific Research (TNO), NL; [2]Brightlands Materials Center, NL, [3]Fundamental Aspects of Materials and Energy (FAME), Faculty of Applied Sciences, Delf University of Technology, NL; [4]Van 't Hoff laboratory for Physical and Colloid Chemistry, Debye Institute for Nanomaterials Science, Utrecht University, NL; [5]Dept. of Applied Physics and Science Education, Eindhoven University of Technology, NL; [6]Eurofins Materials Science BV, NL; [7]Design and Synthesis of Inorganic Materials (DESINe), Institute for Materials Research, Hasselt University, BE

Induction heating is a fast and efficient process, allowing for selective heating through the use of an alternating magnetic field. However, this process is generally limited to the heating of (magnetic) metallic parts.[1] In order to achieve selective heating in non-magnetic, non-metallic materials, ferrimagnetic nanoparticles can be dispersed into the material matrix to act as magnetic susceptors. Such an application can be of interest for (de)bonding on demand (DoD) applications of thermoplastic adhesives, as it allows for more energy efficient bonding and increased recyclability at end of life scenarios.[2] An interesting candidate for such DoD applications is magnetite (Fe_3O_4), an earth-abundant ferrimagnetic material. The magnetic properties of magnetite nanoparticles are dependent on particle size, morphology and phase composition, and need to be optimized to achieve maximum induction heating performance.[3] In this work, octahedral magnetite particles with four distinct particle sizes ranging from 40 to 80 nm in diameter, were synthesized and characterized. The magnetic properties and induction heating performance of the nanoparticles were linked to the material properties. POE was chosen as a model thermoplastic adhesive. As such, the particles were dispersed into a POE matrix, and the inductive heating properties of the Fe_3O_4-POE composite were investigated in order to reach relevant processing temperatures.

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IM - D2 - O05

From prebiotic chemistry to nanostructured materials: One-pot synthesis of multifunctional C-N systems from diaminomaleonitrile for photocatalytic applications

Marta Ruiz-Bermejo[1], Antonio López-García[1], José L. de la Fuente[2], M. Pilar García Armada[3]
[1]Centro de Astrobiología (CAB) CSIC-INTA, ES; [2]Instituto Nacional de Técnica Aeroespacial "Esteban Terradas" (INTA), [3]Escuela Técnica Superior de Ingenieros Industriales, ES

Since 2015, there has been growing recognition that prebiotic chemistry can provide not only insight into early chemical evolution, but also simple and efficient routes for the development of functional materials.[1] Accordingly, starting from single molecular precursors such as sodium or ammonium cyanide salts, and in particular diaminomaleonitrile (DAMN, the tetramer of hydrogen cyanide), our initial work explored how chemically plausible abiotic (hydro)thermal environments can be exploited to generate extended conjugated C–N frameworks through minimal synthetic procedures. These early studies led to the identification of a new family of multifunctional materials, which were evaluated as capacitors, biosensors, semiconductors and catalysts.[2-6]

More recently, and beyond the constraints of prebiotic chemistry, we have demonstrated that DAMN can be efficiently transformed into C–N-rich materials (DAMN-derived polymers) through simple one-pot reactions in alcoholic media.[7] These precipitation-driven processes require neither catalysts nor templates, involve no multistep protocols, and only demand minimal post-synthetic treatment by filtration. Remarkably high, near-quantitative yields are achieved under mild solvothermal conditions (below 150 °C) using environmentally friendly alcohols such as pentanol and hexanol. While DAMN polymerisation in water or in the melt leads to micrometre-sized particles, the use of alcoholic solvents proves particularly advantageous, yielding nanoparticulate materials with enhanced textural properties. This clearly demonstrates that the morphology of DAMN-derived polymers can be tuned through the choice of synthetic conditions.[8] Importantly, all the materials obtained exhibit semiconducting behaviour and have been evaluated as photocatalysts using the photodegradation of the persistent organic pollutant lindane as a proof of concept. The nanoparticulate systems synthesised in alcoholic media show especially promising photocatalytic performance, which is attributed to their reduced particle size and increased accessible surface area.[8]

These results show that high-yield one-pot reactions inspired by prebiotic chemistry can produce advanced functional materials from a single simple precursor, bridging chemical evolution and materials innovation.

This research has been funded by grant No. PID2022-140180OB-C22 by the Spanish Ministry of Science and Innovation/State Agency of Research MCIN/AEI/ 10.13039/501100011033 and by "ERDF A way of making Europe".

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IM - D2 - O06
One-step synthesis of micrometer scale chiral gold materials

Mathias R.S. Nielsen, Miguel A. Ramos Docampo
Interdisciplinary Nanoscience Center (iNANO), Aarhus University, DK

Chirality is an intrinsic feature of natural systems. From the macroscale to the nanoscale, the way materials self-assemble in a mirror-like non-superimposable fashion defines their properties, characteristics and functions. This concept, which has largely been known in biology and extensively used afterwards in pharmacology, is now exploding in the realm of inorganic nanomaterials.[1] Chiral nanomaterials may advance science in the fields of catalysis, sensing and optics. To date, only nanometer scale, chiral materials have been reported, and the methods to produce them are laborious and low yield. We have developed a completely new method to produce high yield, pure and chiral-active micrometer-scale long and nanometer-scale wide chiral gold materials in a one-step and cost-effective process. The method allows for tuning the material topology and handness. Further, this material serves for cell alignment and patterning.[2]

The authors acknowledge The Lundbeck Foundation.

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IM - D2 - O07
Boron-containing phthalonitrile thermosets for enhanced thermal neutron shielding

Oussama Mehelli[1], Nour Elislem Leblalta[1], Abdelmalek Habes[1], Mehdi Derradji[1]
[1]UER Procédés Energétiques, École Militaire Polytechnique, DZ

The development of lightweight polymeric materials with high efficiency toward thermal neutron attenuation is of significant interest for nuclear energy systems, radiation protection, and advanced structural applications. In this study, a boron-containing phthalonitrile thermoset (PN-B) was developed through chemical incorporation of boron into the phthalonitrile monomer, followed by thermal curing to obtain a highly crosslinked polymer network. This molecular-level integration enables a homogeneous boron distribution and enhances neutron capture efficiency compared to conventional filler-based approaches. The synthesized PN-B monomer was structurally characterized using FTIR spectroscopy as well as ^1H and ^11B NMR analyses, confirming successful formation of the phthalonitrile framework and effective boron incorporation. Differential scanning calorimetry was employed to investigate the curing behavior of the monomer, revealing suitable reactivity for thermoset processing. After thermal curing, the resulting PN-B polymer was characterized by FTIR spectroscopy to verify network formation and by thermogravimetric analysis to assess its thermal stability, demonstrating excellent resistance to thermal degradation. The thermal neutron shielding performance of the PN-B polymer was quantitatively evaluated using macroscopic neutron attenuation parameters. The material exhibited a macroscopic cross-section (Σ) of 1.477 cm^{-1} and a mean free path (λ) of 0.469 cm. A high screening ratio of 88.1% was achieved at a thickness of 13 mm, highlighting the strong neutron attenuation capability of the boron-functionalized phthalonitrile thermoset. These results demonstrate that PN-B represents a promising high-performance material for thermal neutron shielding applications requiring both efficiency and thermal robustness.

IM - D2 - O08
ETS-10 coated honeycombs as possible candidate for CO_2 capture in humid flue gas streams

Morgane Van Hove[1,2], Ben Sutens[1], Steven Mullens[1], Guy De Weireld[2]
[1]Flemish Institute for Technological Research (VITO NV), BE; [2]University of Mons, Faculty of Engineering (UMONS), BE

To limit global warming to below 1.5°C, net-zero CO_2 emissions must be achieved by 2050. While reduction of energy consumption and transitioning to renewable energy are essential, it has an insufficient impact in a short-term and worldwide scale.[1] Carbon dioxide removal strategies such as Carbon Capture Utilisation and Storage (CCUS) are therefore critical especially in hard-to-abate sectors.[2] Current industrial CCUS relies on liquid amine absorption, which suffers from high energy demand and solvent degradation.[3] Solid adsorbents offer a promising alternative, yet their CO_2 capacity in humid conditions remains a major challenge.[4]
ETS-10, a titanosilicate zeolite, has shown that it retains its CO_2 uptake under high relative humidity (90% RH) in powder form.[5] However, whether this moisture tolerance is preserved in structured configurations remains unclear. Given its production on kg scale, ETS-10 was selected for structuring on cordierite honeycombs via vacuum wash-coating to assess its dynamic performance under realistic flue gas conditions. Initial characterisation (XRD, SEM-EDX, TGA-MS, N_2 sorption) confirmed material purity and porosity. Firstly, static CO_2 and H_2O isotherms were measured, then dynamic breakthrough experiments revealed more insights in mixed streams. ETS-10 structured on honeycombs demonstrated promising CO_2 uptake under humid conditions, suggesting potential for outperforming conventional zeolites when integration precedes H_2O displacement. However, precise capacity values and direct comparisons remain under investigation due to differences in humidity levels and measurement conditions.[6]
To further reduce moisture effect, cation exchange was explored. Inspired by studies on 13X, Na-ETS-10 was exchanged with H^+, K^+, Ba^{2+}, and Cs^+. Among these, K-ETS-10 exhibited the best balance in retaining CO_2 capacity while reducing H_2O uptake. Protocols to improve K^+ exchange degree were implemented, enabling the production of optimized ETS-10 on a large scale. The material was successfully structured on honeycombs and benchmarked against Na-ETS-10 to evaluate its dynamic performance.
These findings highlight ETS-10's potential as a moisture-insensitive adsorbent for CO_2 capture in humid flue gas streams, offering a scalable and energy-efficient alternative to conventional technologies.

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IM - D2 - O09
Circular lignin epoxies: Activation and functionalisation for BPA-free, self-healing thermosets

Giorgio Tofani[1], Meta Florjančič[1,2], Iva Edrovska[1,2], Rok Pogorevc[1], Marko Gabrovšek[1], Edita Jasiukaitytė-Grojzdek[1], Filipa A. Vicente[1], Miha Grilc[1], Blaž Likozar[1,2]
[1]National Institute of Chemistry, SI; [2]University of Ljubljana, SI

Epoxy thermosets underpin high-performance applications but remain dominated by bisphenol-A monomers and irreversible curing, limiting circularity[1]. Lignin offers an abundant aromatic alternative, and its activation/functionalisation can enable the formation of covalent adaptable networks (CANs), allowing recyclability[2].
Two lignin modification strategies, activation in acid organic/water solvent environments, and single-catalyst cyclic anhydride functionalisation, lead to CANs in BPA-free lignin epoxies with competitive properties and heat-triggered repair.
Lignins from different origins were activated in acid organic/water solvent systems by hydrolysis under various conditions and analysed by FTIR and 2D-NMR before blending and curing with epoxide. In parallel, lignins were fractionated, esterified with cyclic anhydride[3] in THF using a single catalyst, and cured with either short- or long- chain diglycidyl ethers; structures and properties were probed by 31P-NMR, SEC, FTIR, TGA, and tensile/self-healing tests.
Activation increased carbonyl content (C=O band shift/intensification), with water content modulating the extent of activation. In the functionalisation route (proprietary patent LU507032B1/EP4640734A1), hydroxyl-to-carboxyl conversion enabled ester-exchange CANs, delivering $T_{onset} > 350$ °C across resins, tensile strength up to ~40 MPa (“rigid resin”), and elongation to ~63 % (“flexible resin”). Examples are shown in Figures 1 2. Multiple repair cycles were demonstrated: two without and up to four–five with a small addition of fresh epoxide, with an expected mechanical property decrease.

The authors gratefully acknowledge financial support from SIn Research Agency (grant P2-0152) and European Union’s Horizon Europe research and innovation programme under grant agreements No. 101058371 (ESTELLA) and No. 101070302 (HyPELignum).

Fig. 1. Example of “rigid resin”.

Fig. 2. Example of “flexible resin”.

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IM - D2 - O10

Tagging for circularity: Fluorescent tagging of polycondensation polymers to enable efficient sorting and enhancing recycling

Jonas Cassimon[1], Christophe Vande Velde[1], Pieter Billen[1]
[1]*University of Antwerp, BE*

Polycondensation polymers are all around us, in our walls, furniture, cars and appliances. Only a small percentage of these polymers are recycled, primarily into inferior products. These polymers are typically heteropolymer with multiple typically used monomers. It is well-understood that these monomers can be cleaved using various chemical recycling techniques, but complex mixtures are often obtained due to this variety in monomers. To limit the complexity and avoid the difficulty of end-of-pipe purification, the polymers should be sorted prior to recycling. Near infrared sorting is a possibility, but it can lack the precision and specificity when closely related monomers are used. To enable sorting based on the monomer, we propose design-for-circularity by incorporating fluorescent tags in the polymer so that each monomer type can be rapidly and sensitively identified without altering product performance. This allows for improved reactor input engineering, providing more efficient processes and higher purity products. Moreover, it allows for producers to trace their own formulations or materials throughout entire lifecycles, as an integral part of circular economy strategies. This research provides a proof-of-concept that fluorescent tags can be in used polycondensation polymers to identify their monomers without changing the mechanical properties. This is done by testing multiple incorporation strategies, exploring the behavior of fluorophore-based tags in polymer matrices, followed by investigating the properties, stability and recyclability of tagged polymers.

This research is funded by the research foundation Flanders through a predoctoral fellowship (Grant No. 1S09725N).

IM - D2 - O11

Paper made greener: Replacing commercial retention and wet strength additives with nanocellulose-based materials

Elisa Giovanna Faggioli[1], Carlo Punta[1,2], Davide Ghirardello[3], Marc Delgado-Aguilar[4], Alessandro Sacchetti[1,2]
[1]Politecnico di Milano, IT; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM), IT; [3]Mare S.p.A., IT; [4]University of Girona, ES

Recently, papermaking industries are trying provide new, environmentally-benign products to transform established, money-earning processes from fossil-based to bio-based. In particular, the most common strength and retention agents, polyamidoamines (PAE) and polyacrylamides (PAM), constitute a challenge to sustainable development, since they reduce repulperability and recyclability[1]. However, the industry has yet to find new additives that can match the exceptional performances that these fossil-based ones can provide. In this context, cellulose nanofibers (CNFs) are an optimal candidate for the paper supply chain, given their affinity with the matrix, their well-known outstanding properties from tensile strength to high surface area and their environmental friendliness[2]. However, commercially available CNFs present anionic charges on their surfaces, while PAE and PAM work by exploiting their characteristic cationic charges[1].
For this reason, in this work, CNFs were produced combining a chemical pre-treatment (TEMPO-oxidation) with a mechanical one, and then they were further modified to introduce the desired cationic charges (cTOCNFs) with a new environmentally friendly procedure[3]. cTOCNFs were then formulated with or without commercial additives and introduced in the bulk phase of papermaking, alone and in combination with organic acids. This allowed to obtain a library of ready-to-add products with comparable results with respect to cationic polymers (Fig. 1): starting from the same nanocellulose-based material, it was possible to tailor the performance of the final paper product based on the desired target additive (PAE, PAM), by selectively modifying the amount of cTOCNFs and the treatment of the paper sheets. Thus, this study is a considerable first step towards making paper(making) a more sustainable process, by substituting fossil-derived additives with bio-based ones with industrial scalability in mind.

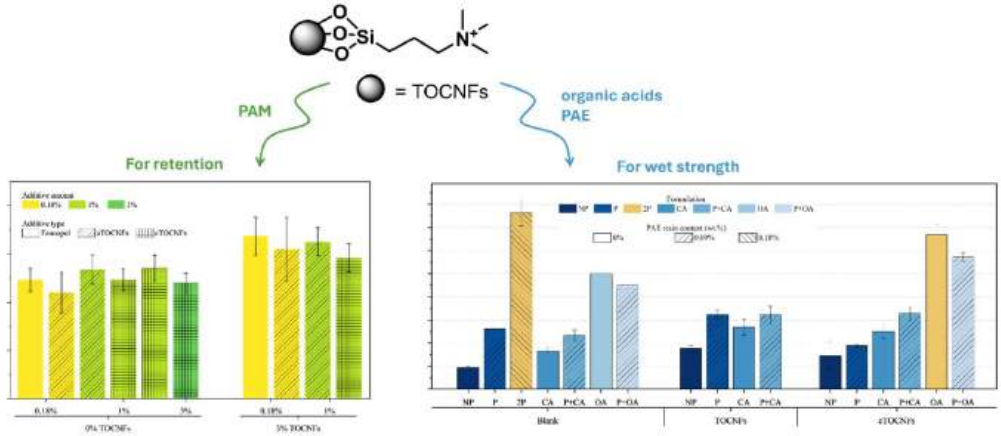

Fig. 1. Graphical abstract of the presented work: on the utilization of cTOCNFs in papermaking as a retention (left) and strength (right) additive with comparable results with respect to commercial additives (overall values on the left, yellow columns on the right)

This study received funding from the European Union NextGeneration EU (National Recovery and Resilience Plan_NRRP): Mission 4, Component 2, Investment 3.3_DM n. 117 02.03.2023. The author wishes to thank Mare SpA as well for financially supporting this study and providing facilities and support throughout.

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IM - D2 - O12

Preserving the past with greener materials: Multifunctional nanocellulose hydrogels and cryogels for cultural heritage conservation

Martina Romani[1], Olivia Gómez-Laserna[1,2], Francesco Caruso[3,4], Erlantz Lizundia[5,6], Maite Maguregui[3,7]

[1]Dept. of Analytical Chemistry, Faculty of Science and Technology, University of the Basque, ES; [2]i+Med S. Coop., Álava Science and Technology Park, ES; [3]Dept. of Analytical Chemistry, Faculty of Pharmacy, University of the Basque Country (UPV/EHU), ES; [4]Conservation Center of the Institute of Fine Arts, New York University, USA; [5]Life Cycle Thinking Group, Dept. of Graphic Design and Engineering Projects, Faculty of Engineering in Bilbao, University of the Basque Country (UPV/EHU), ES; [6]BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU, Science Park, ES; [7]Dept. of Chemical and Biomolecular Engineering, Tandon School of Engineering, New York University, USA

The conservation of cultural heritage faces a critical dual challenge: to ensure the longevity of artworks and minimize the environmental and health footprint of conservation/restoration interventions. Traditional cleaning methods often rely on toxic organic solvents, non-biodegradable synthetic polymers, or single-use materials that generate significant waste. The ENCLOSURE project introduces the development of advanced, bio-based nanocellulose hydrogels and cryogels as high-performance, sustainable alternatives to the above-mentioned traditional methods.

In this paper, we report the synthesis of novel cellulose nanofiber hydrogels designed via green chemistry principles. Unlike conventional gels that employ toxic crosslinkers (e.g., glutaraldehyde), these hydrogels are crosslinked using amino acids such as glycine. This innovation yields biocompatible materials with tunable mechanical properties and unexpected multifunctionality. Experimental results demonstrate their superior efficacy not only in the removal of particulate soiling from easel paintings but also in the complex extraction of copper corrosion patinas (brochantite and atacamite) from bronze objects, outperforming traditional agar-chelating agents systems while providing inherent biocidal activity.

Complementing these hydrogels, we introduce nanocellulose-based cryogels designed for circularity. Reusability of these cryogels allows for the amortization of their production footprint, offering a significantly lower environmental impact compared to standard single-use cleaning agents. Their efficacy in desalinating wall paintings and removing degraded varnishes has been demonstrated.

Our project integrates a pioneering Life Cycle Assessment (LCA) to rigorously assess the sustainability of the proposed materials. Although the use of LCA in this field remains relatively recent, we move beyond standard industrial metrics by defining a heritage-specific functional unit that explicitly accounts for cleaning efficacy per treated surface area. Although production-related issues were identified, the materials' higher efficacy, avoidance of additional fluids, and reuse collectively mitigate their environmental footprint.

Acknowledgements: This work has been supported by the project TED2021-129299A-I00, funded by MICIU/AEI/10.13039/501100011033 and by the European Union NextGenerationEU/PRTR. M. Romani and O. Gomez-Laserna gratefully acknowledge their predoctoral and research contracts, respectively, from University of Basque Country and ENCLOSURE project (TED2021-129299A-I00). F. Caruso acknowledges his Maria Zambrano fellowship from UPV/EHU, funded by the Spanish Ministry of Universities and the European Union NextGenerationEU/PRTR. The authors thank Anna Nualart-Torroja, Africa Pitarch Martí, Tine Frøysaker and Jan Dariusz Cutajar for providing the mock-ups and for their valuable feedback on the performance of the materials and their constructive comments that helped improve the final version of the gels.

IM - D2 - O13

Sustainable preparation of nitrogen-doped carbon dots for improved luminescent sensing

Rut Sisó-Moliné[1], Maria Méndez[2], Maria Cinta Pujol[1], Joan Josep Carvajal[1]
[1]Universitat Rovira i Virgili (URV), Dept. de Química Física i Inorgànica, ES; [2]Institut Català d'investigació Química (ICIQ), The Barcelona Institute of Science and Technology (BIST), ES

Carbon dots (CDs) are zero-dimensional photoluminescent nanomaterials primarily composed of carbon atoms. Their facile and sustainable synthesis, together with their unique optical properties, has attracted considerable interest for applications such as non-invasive luminescent sensing[1]. Bottom-up fabrication of blue–green emitting CDs from commercial small-molecule precursors, including amino acids or monosaccharides[2], has been widely explored. However, two main limitations remain: (i) the reliance on commercial reagents conflicts with green chemistry principles by neglecting bio-waste feedstocks, and (ii) blue–green emission is suboptimal for biological applications, where longer wavelengths are required to improve tissue penetration and reduce light absorption[3].

This work addresses these challenges by employing hemicellulose extracted from almond shell waste as sustainable precursor and by redshifting CD emission through nitrogen doping with ortho-, meta-, and para-phenylenediamine (o-, m-, p-PDA). The resulting CDs were evaluated as luminescent nanothermometers and pH sensors over 298–358 K and pH 1–13.

Hydrothermal synthesis using hemicellulose produced CDs with average size of 3.5 ± 0.9 nm—90% smaller than those from commercial xylose—leading to enhanced photoluminescence with excitation-dependent blue emission under UV light. PDA doping further modulated the optical response: m- and p-PDA yielded excitation-independent green emission, while o-PDA produced dual excitation-dependent bands. Consequently, m- and p-PDA CDs operated as single-band thermometers, whereas o-PDA enabled ratiometric sensing. The best system (50 wt% m-PDA) achieved maximum relative thermal sensitivity of 5.0 % K^{-1} and temperature resolution of 0.2 K at 298 K, demonstrating excellent performance within the biological temperature range.

These results were supported by grant PID2021-128090OB-C22 funded by MICIU/AEI/10.13039 /501100011033/ and FEDER/UE. Additional funding was provided by URV and Diputació de Tarragona through grant 2023PMF-PIPF-24.

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IM - D2 - O14
Hydrazone-based covalent organic frameworks

Bianca A. Paltin[1, 2], Iuliana M. Chirica[1], Mihaela M. Trandafir[1], Mihaela Matache[2], Mihaela Florea[1], Anca G. Mirea[1]
[1]National Institute of Materials Physics, RO; [2]University of Bucharest, Faculty of Chemistry, RO

Covalent organic frameworks (COFs) represent a unique class of crystalline organic polymers that are structurally predesignable, synthetically controllable, and functionally tunable.[1] These materials exhibit highly ordered architectures, permanent porosity, large specific surface areas, and excellent chemical and thermal stability.[2] Over the past decade, the rational design, targeted synthesis, and property optimization of COFs have attracted significant attention, leading to their exploration in a wide range of applications, including photoconductive materials, gas adsorption, drug delivery, heterogeneous catalysis, and chemical sensing.[2]
Herein, we present the synthesis of novel two-dimensional hydrazone-linked COFs with high crystallinity and enhanced optical properties. These frameworks are constructed from simple, well-defined molecular building blocks featuring pyrene cores functionalized with aldehyde and hydrazide groups, derived from terephthalic or trimesic acid, using solvothermal method. The incorporation of additional functional groups, such as hydroxyl (–OH) or tert-butyl (*–tBu*) substituents, is expected to improve solubility and further enhance the optical properties of the resulting materials. The structure and properties of the synthesized COFs were investigated using XRD, FTIR, solid state NMR, and BET. These compounds can be utilized in a range of applications, notably gas adsorption or photocatalysis.

Fig. 2. Design, synthesis and possible topology of hydrazone-based COFs

This work was supported by Romanian Ministry of Research, Innovation, and Digitization through the Core Program 2023–2026 (contract PC3–PN23080303), and AGM, IMC, MMT, BAP, and MF acknowledge the CNCS/CCDI-UEFISCDI for the COFUND-NEXT-PEMFC project, within PNCDI IV.

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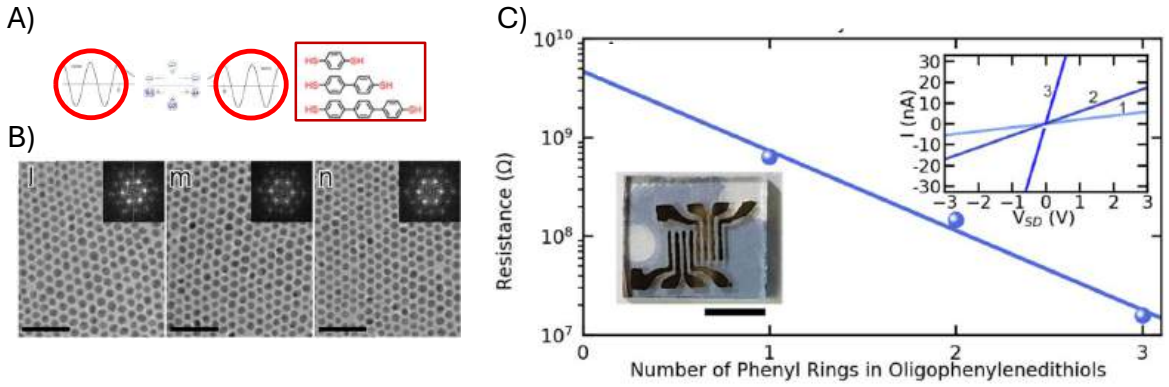
IM - D2 - O15
From nano building-blocks to a new class of 2-D nanosheets

Steven Gravelsins[1], Myung Jin Park[1], Marek Niewczas[2], Seok-Ki Hyeong[3], Seoung-Ki Lee[4], Aftab Ahmed[5], Al-Amin Dhirani[1,6]
[1]Dept. of Chemistry, University of Toronto, CA; [2]Dept. of Materials Science & Engineering, McMaster University, CA; [3]Functional Composite Materials Research Center, Institute of Advanced Composite Materials, Korea Institute of Science and Technology (KIST), KR; [4]School of Materials Science and Engineering, Pusan National University, KR; [5]Dept. of Electrical Engineering, California State University, USA; [6]Dept. of Chemistry, University of Toronto, CA

2D nanosheets, such as graphene and other van der Waals materials that have been isolated from bulk materials, have revealed extraordinary optical and electronic behaviour. An alternate potential approach to fabricate nanosheets - and materials generally - is to employ a bottom-up strategy using nanostructures as building blocks. This approach leads to a possibility of nanoengineering materials (NEMs) potentially exhibiting emergent quantum phenomena (q-NEMS).
Here, we present a bottom-up method to fabricate for the first time highly ordered, molecularly cross-linked nanoparticle sheets (XNS) – see Figure. XNS fabricated with gold nanoparticles and semiconducting linkers (oligophenylene dithiol, HS-$(C_6H_4)_n$-SH, with $1 \leq n \leq 3$) enable macroscopic observation of quantum "molecular wire" behaviour: resistance decreases with increasing molecule length (the opposite trend of tunneling). Also, the nanosheets exhibit strongly enhanced molecular optical absorption compared with those of unlinked molecules in solution. We propose that the enhancement arises from strong molecule – nanostructure interaction.
These results underscore q-NEMS as a viable platform for fabricating a wide range of materials with bottom-up control given the vast number of organic and inorganic nano building blocks available.



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IM - D2 - O16
Polymorphism in 2D HOIPs: Elastic and optical structure–property relationships

Paola La Magna[1], Asli Semerci[1], Ian P. Machado[2], Anna M. Kaczmarek[2], Martijn Mertens[3], Wouter T.M. Van Gompel[3], Kristof Van Hecke[1]
[1]XStruct, Dept. of Chemistry, Ghent University, BE, [2]NanoSensing group, Dept. of Chemistry, Ghent University, BE, [3]Hybrid Materials Design (HyMaD), Institute for Materials Research (IMO-IMOMEC), Hasselt University, BE

Over the past decade, hybrid organic–inorganic perovskites (HOIPs) have attracted considerable interest, mainly due to their use in perovskite solar cells (PSCs).[1] Two-dimensional (2D) HOIPs have gained attention because of their superior stability compared to their three-dimensional (3D) counterparts and enhanced compositional versatility.[2,3] In 3D HOIPs (ABX_3, B = Pb^{2+}, X = I^-, Br^-, or Cl^-), the A-site cation is limited to small organic molecules, whereas 2D HOIPs (A_2BX_4) can also accommodate bulkier cations.
Most reported 2D HOIPs employ simple organic spacers, but their architecture enables the use of more complex cations. In addition, their polymorphism can arise not only from compositional changes but also from crystallization conditions.
Here, we report 2D HOIPs based on 3-phenyl-1-propylamine (PPA), focusing on how crystallization techniques affect structure and properties. Single crystals were obtained via solvent layering and antisolvent vapor-assisted crystallization (AVC). Single-crystal X-ray diffraction (SCXRD) revealed two distinct polymorphic structures (Figure 1).[5,6]

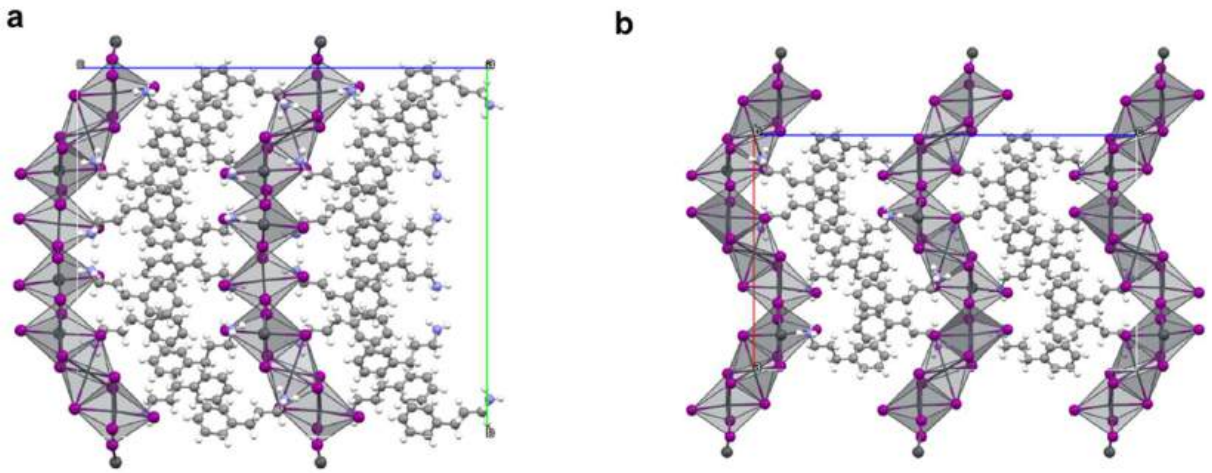

Fig. 1. Crystal structure packing of PPA-based HOIPs using (a) solvent layering and (b) an AVC method.

The polymorphs differ in the connectivity of the inorganic layer: one combines corner- and face-sharing PbI_6 octahedra, while the other consists of corner-sharing Pb_3I_{10} trimers. Despite this subtle difference, their properties differ significantly. The mixed octahedra polymorph exhibits elastic mechanical flexibility and enhanced photoluminescence, compared to the trimer polymorph, highlighting the strong structure–property relationships in 2D HOIPs.

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IM - D2 - O17

Exploring the Er,Yb upconversion system for thermometry in the first biological window

Ian P. Machado[1]*, Andries Meijerink[2], Anna M. Kaczmarek[1]

[1]NanoSensing Group, Dept. of Chemistry, Ghent University, BE; [2]Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, NL

The field of luminescence (nano)thermometry has developed enormously in the past two decades. This technique allows precise and minimally invasive temperature sensing, essential features for real-time biological monitoring, considering that inflammatory conditions and tumors cause local temperature increase.[1,2] In this context, Er^{3+},Yb^{3+}-doped upconversion nanoparticles (UCNPs) have been deeply investigated for ratiometric thermometry. These UCNPs can be excited with near-infrared (NIR) lasers (~980 nm), and the Er^{3+} emissions $^2H_{11/2}\rightarrow{}^4I_{15/2}$ (~520 nm) and $^4S_{3/2}\rightarrow{}^4I_{15/2}$ (~550 nm) arise from the thermally coupled $^2H_{11/2}$ and $^4S_{3/2}$ levels, allowing temperature monitoring in physiological conditions. However, these Er^{3+} emissions are located in the visible range of the electromagnetic spectrum, which is highly absorbed by biological tissues. Therefore, it is important to design materials that fully operate in the biological windows (BWs), namely BW-I (700–950 nm), BW-II (1000–1350 nm), and BW-III (1550–1870 nm).

In this work, we explored the NIR Er^{3+} emissions $^2H_{11/2}\rightarrow{}^4I_{13/2}$ (~780 nm) and $^4S_{3/2}\rightarrow{}^4I_{13/2}$ (~840 nm) (Fig. 1a), located in the BW-I. For this, $NaGdF_4$:Yb18%,Er2% UCNPs of different sizes and morphologies were synthesized, as well as bulk powders, to be investigated as model materials. As these NIR Er^{3+} emissions fall in a region of low sensitivity for standard visible-range PMTs, a systematic investigation of detector systems was performed when studying the luminescent and thermometric properties of these materials (Fig. 1b–d). Distinct spectral profiles were obtained from a single sample, due to the detectors' different responses in the BW-I wavelength range. The effects of such different responses were deeply investigated in terms of fitted ΔE values, relative sensitivities (S_r), and temperature uncertainties (σT). These results highlight the importance of deeply understanding how experimental conditions may alter thermometry results, and could assist researchers in properly selecting detectors for nanothermometers that fully operate in the BW-I spectral region.

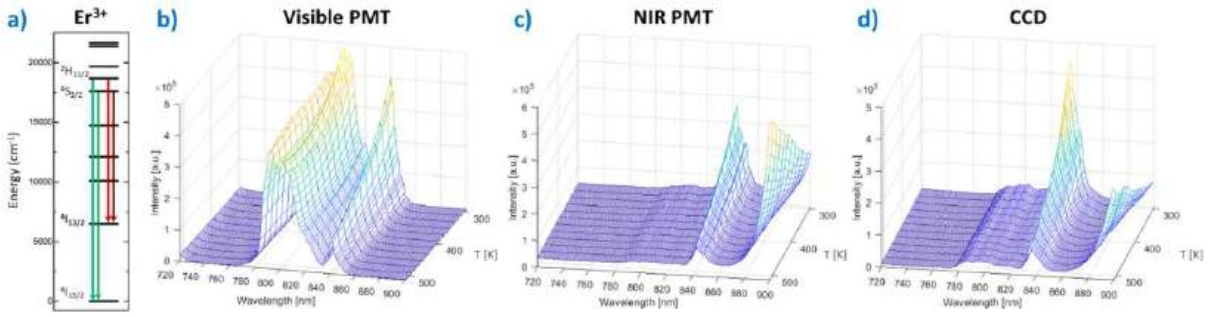

Fig. 1. (a) Energy level structure of the Er^{3+} ion, highlighting its green and NIR emissions.
(b–d) Photoluminescence emission maps with increasing temperature of $NaGdF_4$:Yb18%,Er2% materials recorded using (b) visible-range photomultiplier tube (PMT) detector, (c) NIR-range PMT detector, and (d) charge-coupled device (CCD) detector.

The authors acknowledge the European Research Council (ERC), as this project was developed under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 945945). TEM measurements were performed at the UGent TEM Core Facility.

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IM - D2 - O18

PhotoCORM functionalized nanodiamond particles as a novel tool for targeted tumour therapy

Elisabeth Mayerhoefer[1], Lorena Larios Salazar[2], Himalaya Parajuli[2], Daniela Elena Costea[2], Harsh Nitin Dongre[2], Anke Krueger[1,*]

[1]Institute of Organic Chemistry, University of Stuttgart, DE; [2]The Gade Laboratory for Pathology and Centre for Cancer Biomarkers (CCBIO), Dept. of Clinical Medicine, University of Bergen, NO

Carbon monoxide, a toxic gas, has received much attention as potential therapeutic agent when released at specific sites and in low concentrations. However, dosage and localization of CO administration to reach the targeted cells or tissues has proven very challenging, thereby hampering medical application.[1] This is where CO-releasing molecules (CORMs) come into focus, which deliver CO in a masked way e.g. upon irradiation (photoCORMs) and enable the spatially resolved release over defined periods of time. However, many of these are either insoluble in physiological media or show non-specific toxicity or low bioavailability.

We report on the immobilization of two different photoCORMs on nanodiamond particles for the delivery of CO to cancerous tissues and their investigation as potential therapeutics in vitro and in vivo. Nanodiamond is a promising, highly biocompatible nanomaterial with a rich surface chemistry.[2]

The chosen UV-photoCORM consists of a manganese complex, which has been immobilized together with a small EGFR-targeting peptide to ensure site-specific delivery. The release of CO with spatiotemporal resolution using blue light induced significant cancer specific cytotoxicity with high selectivity. The second, organic NIR-photoCORM can be activated using near-infrared light, which enables deeper tissue penetration and reduces risks of cellular radiation damage. We combined this NIR-photoCORM with nanodiamond for improved stability, bioavailability, and targeting efficiency. We demonstrate the efficient release of CO from NIR-photoCORM functionalized nanodiamond particles using 800 nm light in different physiological media and *in vitro*. Furthermore, biological experiments reveal a remarkably increased amount of dead cancer cells after incubation with ND-photoCORM particles under irradiation. *In vivo* tests additionally show a reduction in tumor volume during treatment with ND-photoCORMs. These results open the way for nanodiamond-based targeted cancer treatments using non-invasive stimuli.

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IM - D2 - O19
Thermally stable binary two-dimensional hybrid organic-inorganic perovskite glasses

Arad Lang[1,2], Chumei Ye[2,3], Celia Chen[2,3], Emily V. Shaw[2,3], Lauren N. McHugh[4], Siân E. Dutton[3], Thomas D. Bennett[2,5]
[1]Dept. of Materials Science and Engineering, Technion – Israel Institute of Technology, IL; [2]Dept. of Materials Science and Metallurgy, University of Cambridge, UK; [3]Cavendish Laboratory, University of Cambridge, UK; [4]Dept. of Chemistry, University of Liverpool, UK; [5]MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Physical and Chemical Sciences, University of Canterbury, NZ

Two-dimensional hybrid organic-inorganic perovskites (2D-HOIPs) have recently garnered significant attention for their potential integration into next-generation optoelectronic applications. Their chemical diversity and straightforward synthesis, together with band gap tunability and enhanced stability, make them promising candidates to replace their three-dimensional counterparts as active materials in photovoltaics, light emitters, and photodetectors.[1] Recent studies have revealed that 2D-HOIPs with the chemical formula $(RNH_3)2MX_4$ (where R is a bulky organic moiety, M is a divalent metal cation, and X is a halide) can undergo melting – a reversible solid-liquid transition – upon heating. Furthermore, by carefully engineering the organic cation, the cooling-induced crystallisation can be suppressed, resulting in a glassy (amorphous) state. However, these so-called "HOIP glasses" exhibit thermal instability, reverting to their thermodynamically stable crystalline form upon mild heating or even at room temperature over a time span of hours to days.[2,3]
In this work, we address the thermal instability of HOIP glasses through melt alloying, a technique we recently demonstrated to apply to meltable 2D-HOIP systems.[4] Binary HOIP glasses were synthesized by blending powders of two glass-forming 2D-HOIPs: $(S\text{-}NEA)_2PbBr_4$ (where S-NEA = (S)-(−)-1-(1-naphthyl)ethylamine)[5] and $(MIPA)_2PbI_4$ (where MIPA = methyl-iodopropylamine).[6] Melt-quenching these blends resulted in the formation of glassy phases. The glass transition temperatures, optical band gap, and mechanical hardness of these glasses were found to depend on the blend composition. Most notably, the binary glasses exhibited complete thermal stability, with no recrystallisation observed even after one month of storage at room temperature.[7]

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IM - D2 - F01

Impact of acceptor strength and backbone planarity on the charge transport of D-A conjugated polymers

Guan-Lin Wu[1], Ting-Yu Wang[1], Po-Te Chen[1], Chu-Chen Chueh[1*]
[1]Dept. of Chemical Engineering, National TW University, TW (R.O.C.)

The development of high-mobility conjugated polymers is crucial for advancing next-generation organic electronics. A key strategy for enhancing charge carrier transport lies in minimizing energetic disorder by enforcing backbone planarity and optimizing intermolecular packing.[1] In this work, we present the design and synthesis of a series of donor-acceptor (D-A) conjugated polymers featuring indacenodithiophene/ dithienopyrrolobenzothiadiazole donor moieties coupled with three distinct electron-deficient acceptor units via an environmentally friendly Aldol condensation procedure (**Figure1**).[2]

Our design strategy focuses on conformational locking, utilizing intramolecular non-covalent interactions (e.g., O···H or S···O bonds) to restrict torsional rotation between monomer units.[3] This approach aims to extend the effective conjugation length and promote ordered $\pi - \pi$ stacking in the solid state. We employ density functional theory (DFT) calculations to thoroughly analyze the nature of these interactions (e.g., O···H vs. S···O) and their influence on the equilibrium main-chain geometry. By systematically varying the acceptor moieties—from a sterically hindered architecture to highly planar, ladder-type configurations—we investigate how subtle structural alterations influence the frontier molecular orbital energy levels, optical bandgaps, and chain assembly behaviors. This design approach enables direct comparison between all-carbon and heteroatom-containing acceptor cores, while elucidating the impact of backbone extension on polymer assembly.

We thoroughly discuss the synthetic routes and comprehensive characterization of these new materials. The influence of backbone rigidity on the thin-film microstructure is analyzed using wide-angle X-ray scattering (GIWAXS) and atomic force microscopy (AFM). Furthermore, their charge transport properties are evaluated in organic field-effect transistors (OFETs). This study provides valuable insights into the structure-property relationships of planar D-A polymers, offering guidelines for designing high-performance organic semiconductors.

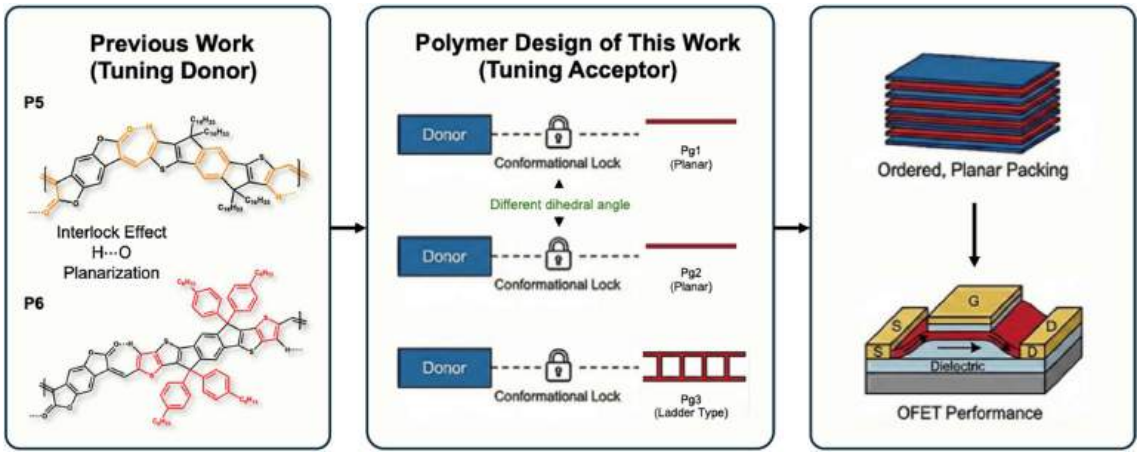

Fig. 1. Design concept of the polymer

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IM - D2 - F02
Applying dissociative chemistry to obtain gradient hydrogels

Brent Van Ballaer[1], Geert-Jan Graulus[1]
[1]Hasselt University, BE

Gradients in the extracellular matrix (ECM) are essential for tissue development, the functioning of the human body, and disease progression, such as in pancreatic cancer (PDAC), where the ECM's mechanical properties correlate with staging of the disease. Studying PDAC in vitro requires models that mimic the mechanical anisotropy of the ECM. We present an innovative approach to create hydrogels with tunable stiffness gradients using dissociative bioorthogonal chemistry.
Our method uses cross-linkers that can be selectively cleaved by a diffusing chemical agent as the external trigger. Controlling the spatial distribution of this cleavage agent allows the formation of continuous stiffness gradients in hydrogels. PEG-based hydrogels were selected as versatile, biocompatible model systems. In depth characterization relates the hydrogels' mechanical properties (obtained via compression testing) to their molecular structure (studied via NMR spectroscopy or derived from gel characteristics) and the reaction kinetics of the studied dissociative chemistry.
This contribution showcases a novel application of dissociative bioorthogonal chemistry. The resulting materials are expected to better emulate the complex tumor microenvironment and may provide a powerful platform for fundamental cancer research by enabling precise studies of how mechanical cues influence tumor development, cellular behavior, and disease progression.

IM - D2 - F03
Cyclodextrin-based sorbents for water remediation

Michal Řezanka[1], Mohamed Ahmed[1], Christopher Hobbs[1], Pavlína Konopáčová[1], Stanislaw Waclawek[1]
[1]Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, CZ

The presence of persistent organic pollutants, such as pharmaceuticals and per- and polyfluoroalkyl substances (PFAS), represents a critical challenge for current water treatment technologies.[1] Cyclodextrins offer a unique supramolecular platform for pollutant removal due to their ability to form stable host–guest inclusion complexes with a wide range of organic contaminants.
This contribution presents an integrated overview of our recent work on cyclodextrin-based adsorptive materials for water remediation, combining molecular-level insight with functional material design. We demonstrate how chemical functionalization and polymerization of β-cyclodextrins enable the preparation of water-insoluble sorbents, including cyclodextrin nanosponges and cyclodextrin-coated polymer nanofibers,[2,3] exhibiting high affinity toward pharmaceuticals and PFAS, including short-chain analogues.
Adsorption experiments are complemented by advanced spectroscopic techniques and isothermal titration calorimetry to elucidate binding mechanisms. In parallel, state-of-the-art quantum chemical calculations with chemical accuracy are employed to correlate experimental thermodynamics with molecular interaction energies. The combined experimental–theoretical approach provides general design principles for cyclodextrin-based sorbents and highlights their potential as efficient and sustainable materials for advanced water treatment.

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic (grant number LUAUS23155).

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IM - D2 - F04
In-situ growth of bilayer COF Heterojunctions for memristor devices

Guangyuan Feng[1], Steven De Feyter[1]
[1]*Division of Molecular Imaging and Photonics, Dept. of Chemistry, KU Leuven, BE*

Monolayer covalent organic frameworks (COFs) are crystalline porous networks with highly tunable molecular structures, mechanical flexibility, and well-defined electronic properties.[1] Their atomically thin nature and chemical programmability make them attractive building blocks for van der Waals heterojunctions, enabling charge transport and storage behaviors that are inaccessible in single-component systems. In particular, bilayer COF heterojunctions provide a unique platform to modulate interlayer coupling, opening new opportunities for resistive switching and neuromorphic device applications. However, the controlled fabrication of bilayer COF heterojunctions remains challenging. Conventional approaches often lack precise control over lattice alignment and chemical compatibility, resulting in interfacial stress, structural defects, and limited crystallinity. In addition, device fabrication typically relies on membrane transfer processes, which reduce yield and introduce contamination, mechanical damage, and device instability. Weak interlayer interactions further restrict charge transport, leading to low switching ratios, high power consumption, and poor endurance in COF-based memristors.

Here, we propose an in-situ strategy for the construction of bilayer COF heterojunctions, coupled with a transfer-free device integration route. Bilayer COFs will be synthesized at liquid–solid interfaces, while their nucleation and growth will be monitored in real time using in-situ scanning tunneling microscopy (STM), enabling precise control over crystallinity and interfacial coupling.[2] Memristor devices will be directly fabricated on highly oriented pyrolytic graphite (HOPG) substrates, eliminating transfer steps and maximizing interlayer charge transport. By systematically correlating heterostructure design with electrical performance, the work will clarify the intrinsic relationship between interlayer interactions, band structure modulation, and memristive behavior. These insights will advance the rational design of functional 2D polymer heterojunctions and support their application in next-generation neuromorphic and flexible electronic devices.

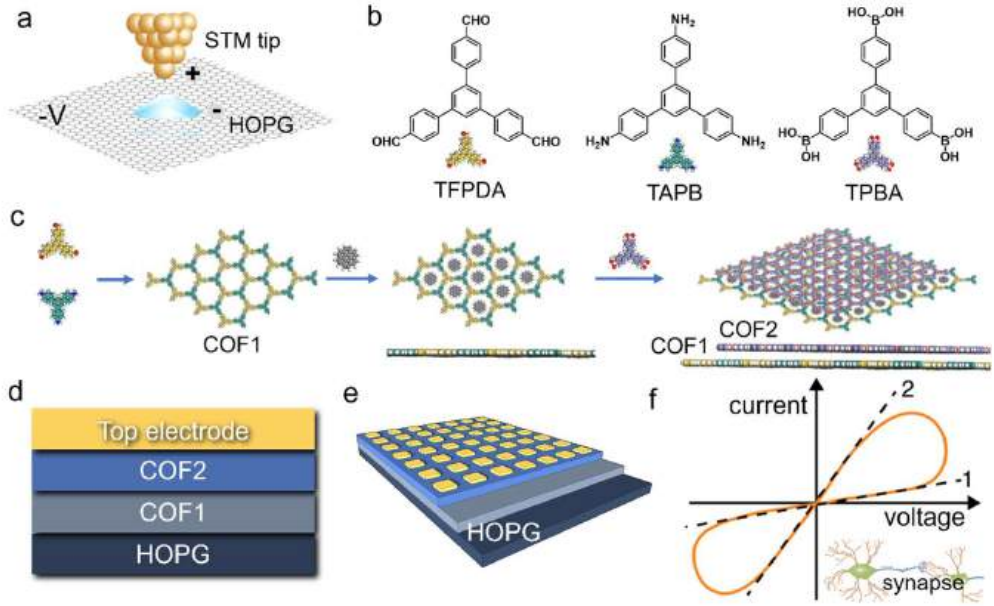

Fig. 1. *(a) STM measurement setup on HOPG substrate. (b) Molecular structures of TFPDA, TAPB, and TPBA. (c) Schematic formation of COF1 and COF2 bilayers. (d) Device architecture: HOPG/COF1/COF2/top electrode. (e) Illustration of COF-based device array. (f) Typical I–V hysteresis loop, indicative of synaptic-like behavior.*

Acknowledgements: Financial support from the Research Foundation-Flanders (FWO VS04526N) and KU Leuven–Internal Funds (C14/19/079) is acknowledged.

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IM - D3 - O01

Nanoscale strain-engineering controls hydrogen reactivity in nanoparticle catalysts

Just P. Jonasse[1], Kaifeng Zheng[2,3], Robin van der Kruit[1], Michael Wilms[4], Jan-Willem Lankman[1], Weixuan Huang[2,3], Mathilde Luneau[4], Petra E. de Jongh[1], Nongnuch Artrith[1], Anatoly I. Frenkel[2,3], Jessi E.S. van der Hoeven[1]

[1]Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands; [2]Dept. of Materials Science and Chemical Engineering, Stony Brook University, USA; [3]Chemistry Division, Brookhaven National Laboratory, USA; [4]Applied Chemistry, Dept. of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, SE

Metal nanoparticle catalysts are the key enablers of sustainable chemical production, with their performance being dictated by their structure. Local deformation or strain at the nanoparticle surface significantly alters the adsorption/desorption equilibria of reactants and intermediates and offers a way to induce different catalytic reactivities in metals than they would exhibit in their unstrained form[1,2]. DFT calculations suggest that for common reactants tensile strain increases binding strength, while compressive strain weakens it[3]. However, experimental verification is complicated due to the lack of well-defined strain-controlled systems. Predominantly bimetallic core-shell nanoparticle systems have been explored that either exhibit tensile or compressive strain but cannot be tuned from one to the other. Furthermore, incomplete core–shell formation and thermally induced intermixing are often encountered problems, obscuring direct correlations between strain and catalytic performance.

In our work, we introduce a novel material system consisting of trimetallic Pt-shell $Au_{1-x}Cu_x$-core nanoparticles (Figure 1a,b)[4]. By changing the Au/Cu ratio in the core, the strain in the Pt shell could be varied from -3.62% compressive (Cu-rich), to +3.79%, tensile (Au-rich) strain (Figure 1c)[4]. Through selected-area electron- and X-ray diffraction, and high-resolution electron microscopy, we quantified lattice strain in our material on multiple length scales. We evaluated the influence of these strain variations on the hydrogen-deuterium isotopic exchange reaction and observed a direct correlation between the hydrogen dissociation activity and lattice strain (Figure 1d), with the highest activity for the tensile strained samples. Our results experimentally validate the theoretically predicted strain–adsorbate relationships and demonstrate lattice strain as a powerful and general design parameter for controlling hydrogenation catalysis.

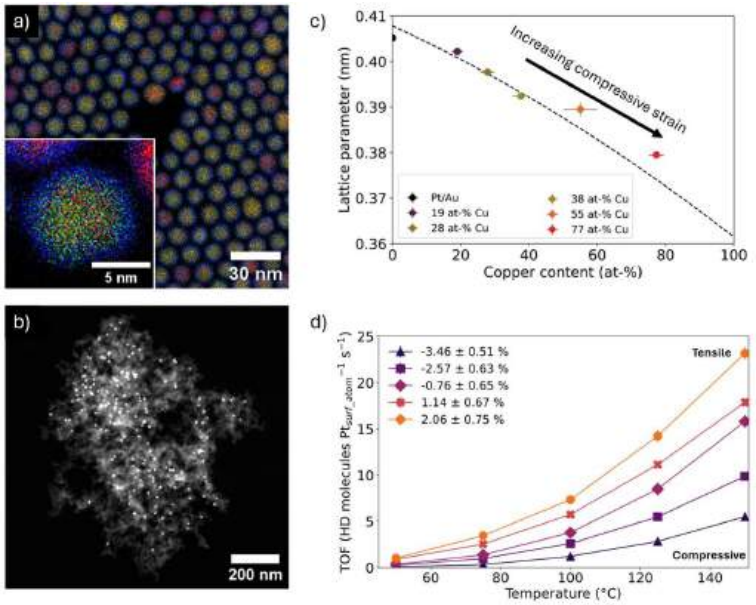

Fig. 1. Overview of our Pt-shell $Au_{1-x}Cu_x$-core nanoparticle system and its performance in HD exchange.
a) STEM-EDX image of unsupported core-shell nanoparticles where Pt, Au and Cu are represented by blue, red and green respectively. b) HAADF-STEM image of supported nanoparticles well-dispersed across the SiO_2 support. c) Graph of the lattice parameter as determined by XRD plotted against the copper content of the core, showing a decrease in lattice parameter with increasing copper content. d) Turnover frequency plotted against temperature for strained catalysts, showing an increase in activity with increasing tensile strain.

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IM - D3 - O02
Strain-modulated hydrogen-deuterium exchange over Au-Pd core-shell nanocatalysts

Jan-Willem Lankman[1], Marta Perxés Perich[1], Xihan Liu[2], Philippe Sautet[2], Jessi E. S. van der Hoeven[1]
[1]Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, NL; [2]Dept. of Chemical and Biomolecular Engineering, University of California, USA

Hydrogen dissociation is an essential step in hydrogenation catalysis and critical to the catalyst performance.[1,2] Recently, Au-Pd core-shell nanoparticle catalysts have emerged as a novel and highly promising class of materials for hydrogenation catalysis.[3] Yet, fundamental understanding on the origin of bimetallic synergy in these core-shell catalysts and their interaction with hydrogen is largely unknown. Here, we investigate the kinetics of hydrogen dissociation and recombination over Au-Pd core-shell catalysts using the hydrogen-deuterium (HD) exchange reaction. We employed colloidally prepared core-shell nanorod catalysts and used 4D scanning transmission electron microscopy to assess the degree and directionality of the strain in the Pd-shell. This revealed that even relatively thick Pd-shells were highly strained in the direction parallel to the surface. Catalytic testing showed that the HD exchange rate increases with increasing Pd-shell thickness and drastically decreases upon alloying. The large increase in apparent activation energy and pre-exponential factor upon alloying indicated a change in rate-limiting step from recombinative desorption to dissociation limited. Interestingly, the core-shell nanorods showed temperature-dependent apparent activation energies and pre-exponential factors, indicating the presence of hydrides in the Pd-shell at the lower temperatures and gradual hydrogen release upon heating which we further substantiated through DFT calculations. Our combined experiment-theory approach revealed that lattice strain and hydride formation can significantly influence the hydrogen dissociation behavior of Au-Pd core-shell nanoparticles, and is relevant to further advance the design of core-shell materials for hydrogenation catalysis.

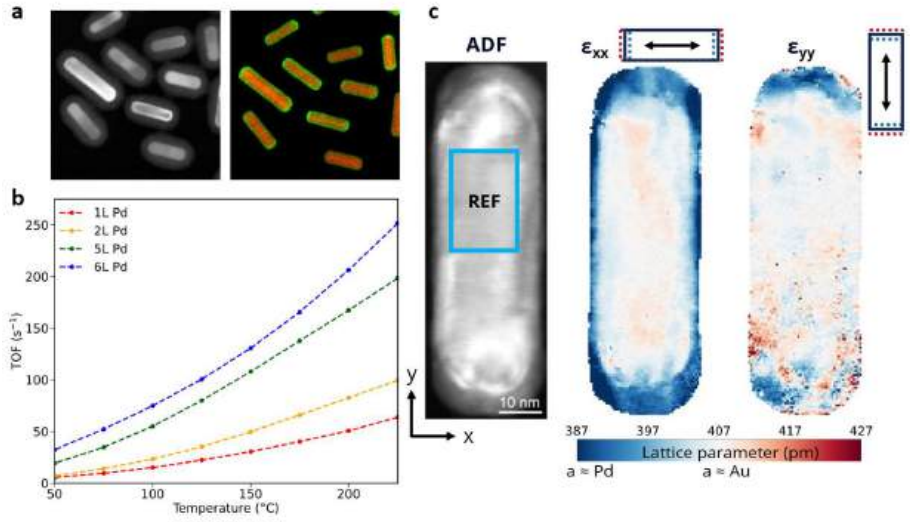

Fig. 1. Shell thickness dependent HD exchange activity over core-shell Au-Pd nanorods. a) annular dark field (ADF) and energy dispersive x-ray spectroscopy (EDX) of core-shell nanorods with 5 layers of Pd, showing the mesoporous silica shell and core-shell structure respectively. b) Turnover frequencies of the nanorod catalysts with different Pd layer thicknesses in the HD exchange reaction. c) 4D-STEM strain analysis of a nanorod including an (ADF) image and the corresponding strain maps in x and y direction.

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IM - D3 - O03

Rationalizing compositional effects of high entropy alloy nanocrystals on electrocatalysis

Jennifer Hong[1], Loredana Protesescu[2], Paolo P. Pescarmona[2], Gianvito Vilé[1,*]
[1]Politecnico di Milano, IT; [2]University of Groningen, NL

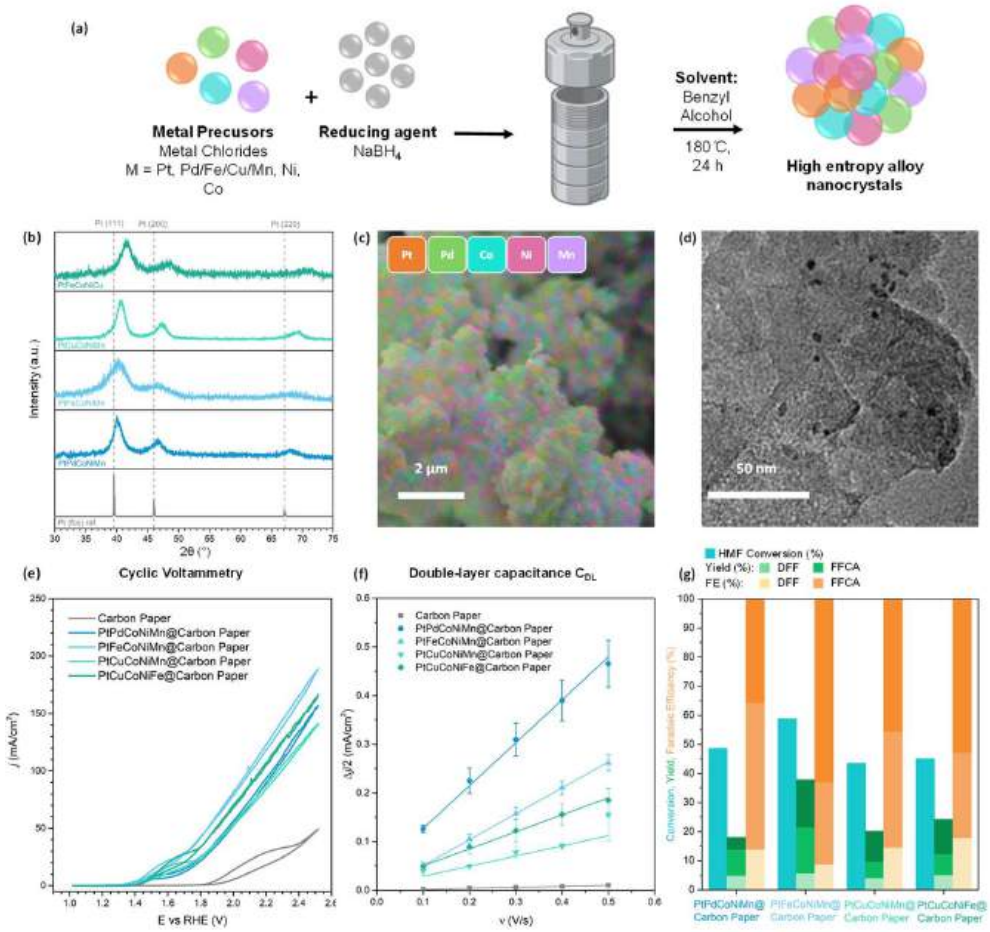

Fig. 1. (a) Schematic representation of the high-entropy alloys nanocrystal synthesis process. (b) XRD patterns of the four synthesized HEAs: PtPdCoNiMn, PtFeCoNiMn, PtCuCoNiMn, and PtCuCoNiFe. (c) SEM-EDAX analysis of PtPdCoNiMn nanocrystals powder. (d) TEM image of PtFeCoNiMn@carbon paper. (e) Cyclic voltammetry of the different HEAs nanocrystals supported on carbon paper recorded at scan rate of 10 mV/s in 1.0 M KOH (pH 13.9) with 100 mM HMF. (f) Difference of anodic to cathodic current density plotted against the scan rate. From the value of slope of the plots (C_{DL}), the double layer capacitance can be calculated. (g) Conversion, yield, and FE of 5-HMF oxidation catalyzed by HEA@carbon paper in 1.0 M KOH at 1.5 V vs RHE for 3 h with 100 mM HMF.

High-entropy alloys (HEAs), composed of multiple elements in near-equimolar ratios randomly distributed within a crystalline lattice, offer a versatile platform for catalyst design.[1] Through compositional tuning, HEAs enable synergistic multimetal interactions and diverse surface atomic environments that regulate geometric and electronic structures, enhancing catalytic performance.[2,3] Lattice distortion, charge redistribution, and tunable d-band centers optimize adsorption energies and reaction barriers, while high entropy and sluggish diffusion impart excellent thermal and chemical stability. Despite these advantages, key challenges remain, particularly in understanding the complex synergistic interactions that govern catalytic performance. In this work, we report the synthesis of HEA nanocrystals with varying metal combinations (PtCoNiM^{1}M^2, M^1, M^2 = Fe, Cu, Mn, Pd) and evaluate their corresponding catalytic activity for the electrochemical oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA). Four HEAs (PtPdCoNiMn, PtFeCoNiMn, PtCuCoNiMn, and PtCuCoNiFe) were synthesized *via* a simple and scalable solvothermal method by reducing five equimolar metal chlorides with $NaBH_4$ in benzyl alcohol at 180 °C for 24 h. Structural and compositional analyses (XRD, XRF, SEM-EDAX, and TEM) confirmed the formation of nanocrystalline HEAs (average particle sizes ~5–6 nm) (fig.1a-c). Electrocatalytic performance of HEAs supported on carbon paper was

evaluated in electrochemical HMF oxidation (100 mM) under alkaline conditions (pH 12.9-13.9 at 1.5 V vs RHE). Electrochemical and HPLC analyses identified PtCuCoNiFe as the most active catalyst at pH 12.9 and PtFeCoNiMn at pH 13.9, demonstrating composition-dependent activity (Fig.1e-g). All HEAs exhibited exceptional selectivity, achieving 99.9% Faradaic efficiency over the competing oxygen evolution reaction. Comparative studies of parent metals and double-layer capacitance (Fig.1f) measurements provided insights into how multimetal interactions influence electronic structure and catalytic behavior in the reaction.

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IM - D3 - O04

A novel coordination polymer made from lanthanide nodes and ferrocene-based linkers with notable hydrogen evolution reaction activity

Marc Morant-Giner[1], Rubén Vázquez-Cárdenas[1], Piotr W. Zabierowski[1], Rui Gusmão[1], Zdeněk Sofer[1]
[1]*Dept. of Inorganic Chemistry, University of Chemistry and Technology Prague, CZ*

Coordination polymers (CPs) are crystalline solids made from metal ions (or cluster centres) and polytopic organic ligands.[1] The possibility of combining properties coming from the building blocks holds the key for the preparation of a plethora of advanced materials.[2]

CPs have been tested as electrocatalysts for water splitting.[3] In this scenario, it has been reported that the integration of ferrocene-containing ligands into highly ordered structure facilitates the electron transfer to the catalytic active sites (usually transition metal elements).[4,5,6] However, very little attention has been paid to the effect of the interaction between lanthanide nodes and ferrocene derivatives on the final hydrogen evolution reaction (HER) activity of CPs.

In this presentation, the synthesis and characterisation of a novel CP containing lanthanide nodes and ferrocene-based linkers will be described. Interestingly, at a current density of 10 mA·cm^{-2}, this material delivered a HER overpotential of ≈200 mV (Fig. 1).

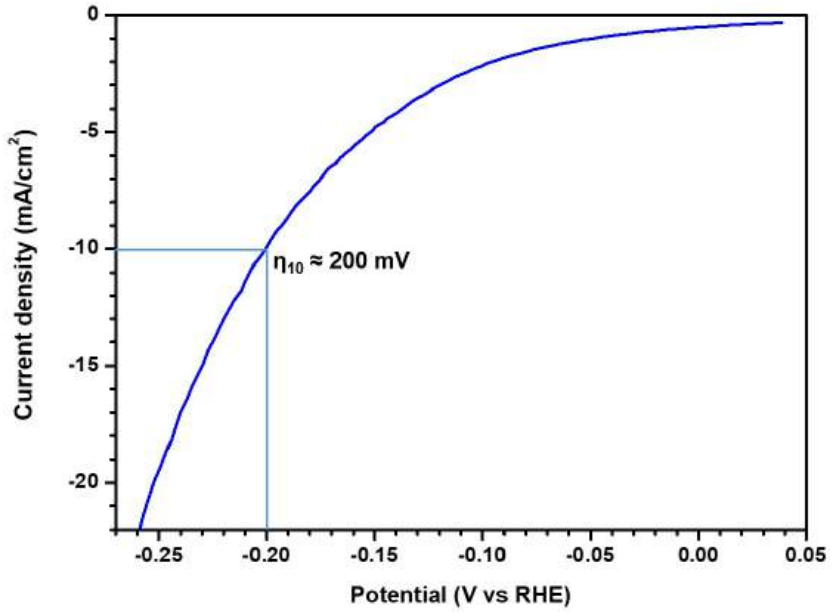

Fig. 1. Polarization curve of the novel CP.

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IM - D3 - O05
Single-atom chemistry on functionalized graphene platforms

Michal Otyepka
Czech Advanced Technology and Research Institute (CATRIN), Palacký University Olomouc, CZ, IT4Innovations, VSB – Technical University of Ostrava, CZ

The isolation of a single graphene sheet transformed nanomaterials research and opened entirely new scientific directions. Although graphene exhibits exceptional electronic mobility, mechanical robustness, and thermal conductivity, its full potential in sensing, biointerfaces, and catalysis can only be realized through deliberate control of its surface chemistry. Covalent functionalization provides a powerful means to modulate graphene's electronic structure, magnetism, and interfacial behavior, however, direct chemical modification of graphene is intrinsically challenging due to its chemical inertness. This limitation is overcome by the chemistry of fluorographene (FG). FG is readily obtained from commercially available graphite fluoride and undergoes reactions under mild and well-controlled conditions, enabling access to a broad library of graphene derivatives that emerge as discrete nanoflakes with well-defined chemical functionalities.[1]
These materials already underpin a wide range of applications, including supercapacitor electrodes,[2,3] lithium-ion[4] and lithium–sulfur[5] batteries, chemical sensing,[6,7] and catalysis.[8–11] A representative example is graphene acid,[12] which functions as an efficient metal-free catalyst for alcohol oxidation. Beyond metal-free systems, FG-derived graphene platforms also serve as ideal anchors for isolated metal species.[8] Cyanographene, bearing nitrile functionalities, stabilizes copper at the single-atom level in mixed valence states and exhibits outstanding activity in dioxygen-driven transformations, including oxidative amine coupling and the selective activation of benzylic C–H bonds to form valuable pharmaceutical intermediates.[10] To further tailor metal coordination environments, we developed graphene supports functionalized with 1,10-phenanthroline-5-amine units, creating well-defined chelating pockets that enable rational and selective placement of transition metals. On this platform, copper sites remain atomically dispersed and display excellent performance in benchmark cross-coupling reactions.[13] Finally, single-atom engineering on carboxylated nitrogen-doped graphene unlocks an unexpected biological function of manganese, yielding a potent, broad-spectrum antibacterial material.[14]
Overall, FG chemistry transforms an inert carbon sheet into a programmable surface, establishing graphene as a modular platform for precise single-atom control and extending its applications.

The work was supported from ERDF/ESF project TECHSCALE (No. CZ.02.01.01/00/22_008/0004587).

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IM - D3 - O06
Intergranular chemistry inside metal oxide compacts and sintering

Oliver Diwald[1], Korbinian Aicher[1], Thomas Schwab[1], Gregor Zickler[1]
[1]Dept. of Chemistry and Physics of Materials, Universität Salzburg, AT

Composite metal oxide nanoparticles are typically far off their thermodynamic equilibrium state.[1] They represent a versatile but so far overlooked source for ceramics, since the intergranular solid-state chemistry can be employed for engineering microstructure and functional properties. We explored the potential of vapor phase-grown MgO nanoparticles hosting Ba^{2+}, In^{3+} and Fe^{3+} admixtures as precursors for engineered intergranular regions.[2,3] Admixed Ba^{2+} ions, either isolated and individualized or as nanocrystalline BaO segregates that decorate the inner pore surfaces give rise to bright and characteristic photoluminescence emissions in the range of visible light.[3]
Moreover, we demonstrated how the admixture of Fe^{3+} and In^{3+} ions to MgO nanoparticles can be used to engage ion exsolution, phase separation, and subsequent spinel formation inside the network of diamagnetic and insulating MgO grains.[2] Extremely high uniformity in the distribution of intergranular ferrimagnetic $MgFe_2O_4$ films and grains with resulting magnetic coercivity values is achieved. Moreover, percolating networks of semiconducting $MgIn_2O_4$ are derived from MgO nanoparticles with admixtures of 20 at% In^{3+} and gives rise to a dc conductivity enhancement by more than five orders of magnitude.[2]

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IM - D3 - O07

Copper-modified hydroxyapatite surfaces as catalysts in environmental processes: A computational perspective

Paolo Fichera[1], Stefano Pantaleone[1], Sebastiano Campisi[2], Antonella Gervasini[2], Marta Corno[1]
[1]Dept. of Chemistry, Interdepartmental Centre NIS, Università di Torino, IT; [2]Dept. of Chemistry, Università degli Studi di Milano, IT

In recent years, hydroxyapatite (HA, Ca10(PO4)6(OH)2) has emerged as a promising material in green chemistry, owing to its feasible synthesis from waste-derived resources. 1 Its tunable acid-base properties, non-toxicity, adsorption capability, and ion-exchange behaviour, make HA an attractive support for eco-friendly heterogeneous catalysts aimed at the abatement of environmental pollutants. 2 In this context, the nature and strength of molecule-surface interactions play a key role in determining catalytic performance. Computational methods have therefore become an essential tool to accurately describe these interactions and to support rational catalyst design, 3 benefitting from the continuous advancement in computational power. 4
In this contribution, a periodic quantum mechanical approach is employed to investigate the interaction between small reactive molecules and the most stable hydroxyapatite surfaces. Copper-modified HA models are considered to enhance catalytic activity while preserving the structural integrity of the material. 5 Specifically, the interaction of formaldehyde, taken as a benchmark volatile organic compound, with the (001), (010), and (101) HA facets is analysed for both pristine and Cu-substituted surfaces. In addition, ammonia selective catalytic reduction (NH_3-SCR) is examined in comparison with experimentally driven data, with particular attention to the effect of water. Variations in structural, energetic, and vibrational properties are discussed to establish a computational framework for the investigation of environmentally relevant catalytic processes. This approach can be readily extended to other cationic substitutions, such as iron, highlighting hydroxyapatite as a versatile and highly promising material for environmental catalysis.

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IM - D3 - O09

Boosting room-temperature lithium-ion conductivity in lithium phosphide and antimonide above 40 mS/cm

Thomas Fässler[1]
[1]*Technical University of Munich, TUM School of Natural Sciences, DE*

Superionic conductors as solid-state electrolyte materials are essential for all-solid-state lithium-ion batteries. Sulfide-based compounds reach in the optimized, rather complex material $Li_{9.54}[Si_{0.6}Ge_{0.4}]_{1.74}P_{1.44}S_{11.1}Br_{0.3}O_{0.6}$ at RT an ionic conductivity of 32 mS/cm.[1]
In recent years we have reported on a design principle for fabricating new superionic conductors based on the very simple structure of Li_3P. Li substitution in Li_3P by *Tr* (*Tr* = Al, In Ga) and *Tt* (*Tt* = Si, Ge, Sn) according to the empirical formula $Li_{3-3x}Tr_xP$ and $Li_{3-4x}Tt_xP$ lead for x= 0.25 to Li_9TrP_4 and Li_8TtP_4 as well as for x = 0.167 to $Li_{14}TtP_6$ and reach Li ion conductivity values up to 4.5 mS/cm. All compounds comprise discrete tetrahedral $[TrP_4]^{9-}$ and $[TtP_4]^{8-}$ units.[2,3]
We report now on transition metal incorporation in Li_3P and Li_3Sb which results in a tremendous increase of the ion conductivity. Sc incorporation in Li_3P results in an increase of the ionic conductivity by four orders of magnitude at a low electronic conductivity. Sc incorporation in Li_3Sb results in a tremendous decrease of electronic conductivity and occurrence of a superionic Li conductivity of 42 mS/cm, thus forming a mixed ionic-electronic conductor.[4]
Crystalline materials are obtained by ball mill synthesis from the elements followed by moderate thermal treatment and are structurally characterized by X-ray and/or neutron diffraction methods. Li ion mobility is investigated by temperature dependent NMR and electrochemical impedance spectroscopy. The role of Li occupation in the various tetrahedral and octahedral sites of the cubic closed packing of P/Sb atoms is highlighted.

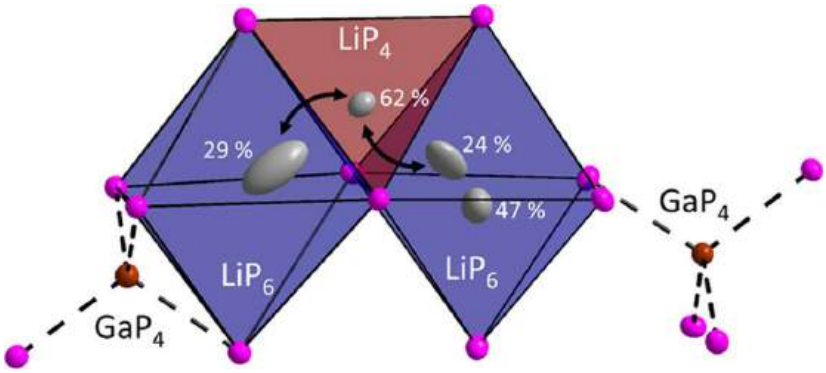

Fig. 1. Structure detail of an example of a of a chalcogenide-based lithium ion conductor indicating the Li ion migration pathway.[3]

Acknowledgements: This work was supported by the Bavarian Ministry of Economic Affairs, Regional Development, and Energy within TUMint.Energy Research GmbH.

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IM - D3 - O10
Electrosynthesis of molecular cluster assembly materials with hierarchical porosity

Lara-Pauline Faden[1], Tom Althaus[2], Karen C. Bustillo[3], Natsuko Asano[4], Shunsuke Asahina[4], Shannon W. Boettcher[1,5], Alexander Katz[1]
[1]Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley, USA; [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), DE; [3]National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA; [4]SMBU, JEOL, Akishima, Tokyo, JP, [5]Department of Chemistry, University of California, Berkeley, USA

We report an electrochemically mediated assembly strategy that couples N-heterocyclic carbene (NHC)–protected tetrairidium clusters into one-dimensional oligomeric chains via direct metal–metal bonds, yielding self-assembled extended architectures with lengths of several nanometres. The hallmark is synthesis of these architectures with the molecular integrity of the individual clusters preserved. We demonstrate this approach across different cluster platforms starting with calix[4]arene-phosphine-protected triruthenium clusters, which are selected for their known propensity toward ring-opening reactions.[1] This concept is generalized with the attachment of a calix[4]arene-functionalized NHC ligand to a tetrairidium core[2,3] produces a hierarchically porous material. We demonstrate that the resulting molecular cluster assembled materials (MCAMs) exhibit emergent macroscopic properties that are highly dependent on the nature of the organic ligand, featuring interconnected pores with dimensions of several hundred nanometres and ultrathin walls down to 5 nm. Notably, the walls themselves are nanoporous, leading to a multiscale porous architecture that bridges molecular, nano-, and mesoscale organization. This approach provides a versatile bottom-up route to hybrid organic–metal materials from discrete molecular clusters, opening new opportunities for designing functional porous materials with tuneable structural and chemical properties relevant to catalysis and other functions relying on high exposed surface areas.

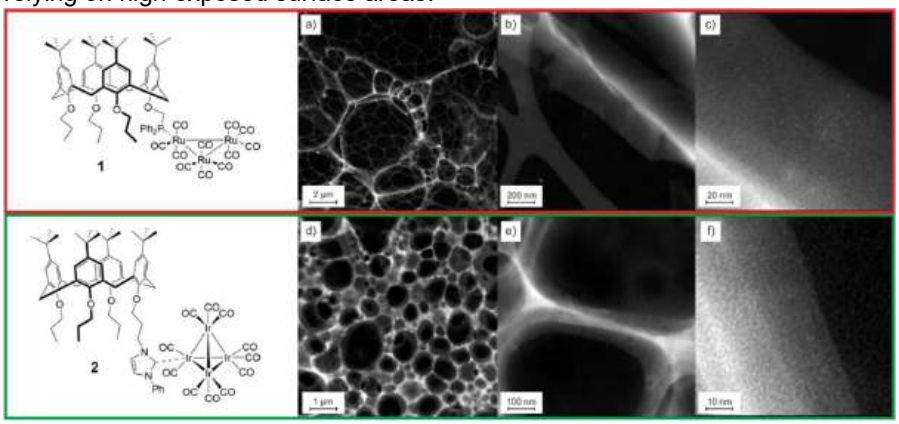

Fig. 1. Starting triruthenium cluster phosphine-complex 1 and starting tetrairidium cluster NHC-complex 2 with HAADF-STEM images with different magnifications of the MCAMs consisting of 1-red (a-b), and 2-red (d-f).

The authors acknowledge financial support from the DAAD through a PROMOS grant. This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Grant No. DE-FG02-05ER15696. Electron microscopy was carried out at the National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. The authors thank Zhongrui Zhou for ESI-MS measurements and Nick D'Antona for providing Pt/Ti-coated glass substrates.

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IM - D3 - O11

Biopolymer-based solid electrolyte membranes for sustainable electrochemical energy devices

Paula Barbosa[1], Sónia A. O. Santos[2], Ana Barros-Timmons [2], Sónia P. M. Ventura[2], Filipe Figueiredo[1]
[1]CICECO – Aveiro Institute of Materials, Dept. of Physics, University of Aveiro, PT; [2]CICECO – Aveiro Institute of Materials, Dept. of Chemistry, University of Aveiro, PT

The pursuit of novel and environmentally friendly materials is crucial for mitigating greenhouse gas emissions and supporting the objectives outlined in the 2030 Agenda for Sustainable Development in the fight against climate change.

Electrochemical energy storage and conversion (EESC) devices present a viable pathway, as they efficiently capture and utilize energy from renewable sources such as solar and wind. However, EESC systems heavily rely on components that are neither renewable nor sustainable, posing significant challenges. The integration of biomaterials into EESC devices offers numerous benefits over conventional materials, including biodegradability, non-toxicity, and cost-effectiveness.

In recent years, our research has been dedicated to exploring these sustainable materials to develop solid-state electrolytes for lithium-ion and sodium-ion batteries, electrochromic devices, and fuel cells. Our primary focus is on solid-state devices, which replace the flammable liquid electrolytes commonly used in conventional batteries with solid polymer electrolytes, thereby enhancing safety and providing greater design flexibility. This technological advancement has significant potential not only for applications in electric mobility but also for stationary energy storage systems, with performance goals targeting energy densities of 450-500 Wh/kg and ionic conductivities surpassing $1x10^{-3}$ S/cm.

This work presents our research on the potential of biopolymer membranes as sustainable solid-state electrolytes for electrochemical applications, such as batteries, electrochromic devices, and fuel cells. These bio-based electrolyte membranes exhibit ionic conductivities reaching 0.03 S/cm, along with remarkable thermal stability, placing them among the most efficient ionic conductors available. Consequently, these innovative materials pave the way for safer and more sustainable energy storage technologies.

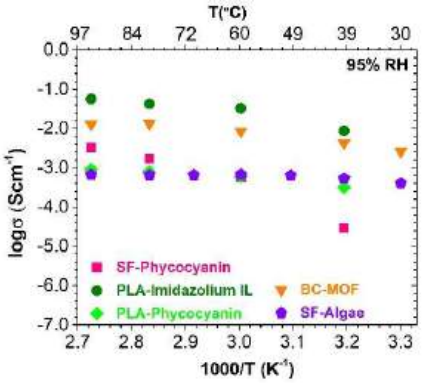

Fig. 1. Biopolymers as polymer electrolyte membranes.

Acknowledgements: This work was financed by the BioEESC project (COMPETE2030-FEDER-00779500) and within the scope of the project CICECO-Aveiro Institute of Materials, UID/50011 & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC), financed by national funds through the FCT/MCTES (PIDDAC). Acknowledgments are also due to FCT/MCTES for the P. Barbosa (2023.06523.CEECIND) contract.

IM - D3 - O12
When frameworks breathe: Soft MOFs for light-driven, self-cooling energy storage

Kezia Sasitharan[1]
[1]*School for Natural and Environmental Sciences, Newcastle University, UK*

The rapid expansion of data-centric technologies has exposed a fundamental materials challenge: energy storage systems dissipate heat faster than conventional cooling infrastructures can sustainably remove it. Breathing metal–organic frameworks (MOFs) such as MIL-53-type lattices exhibit large, reversible structural responses to guest molecules, yet these dynamic degrees of freedom are rarely exploited in energy storage.[1] In my talk, I will demonstrate that soft MOFs with flexible linkers and defect-tolerant architectures can be transformed into active regulators of both charge and heat when coupled to electrolytes tailored to their pore chemistry and mechanical compliance. The system integrates a mechanically compliant MOF network with a photoactive, ionically conductive electrolyte engineered to interact strongly with the framework's pore chemistry and flexibility.[2,3]

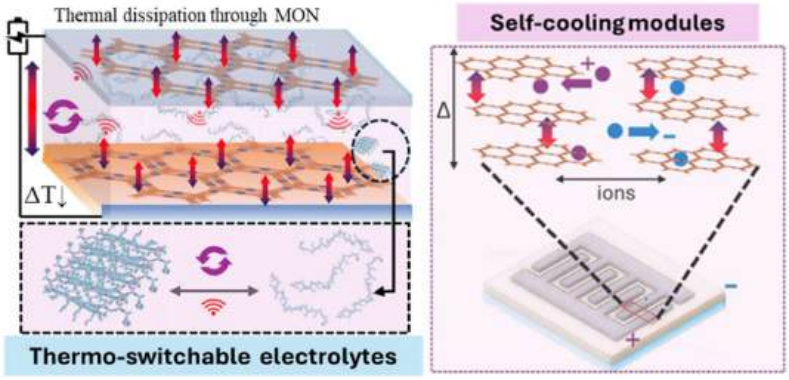

Fig. 1. Thermo-adaptive module: Molecular design enabling reversible folding-unfolding transitions that absorb and release heat, acting as intrinsic molecular thermostats in the energy storage system.

Under illumination, photo-induced charge separation within the electrolyte-MOF interface drives ion redistribution and storage, while the framework's soft structural degrees of freedom activate reversible solvent reorganization and entropy-driven heat dissipation. Photo-electrochemical measurements combined with thermal mapping reveal that illumination enhances charge storage while suppressing local temperature rise during operation. This coupled electrochemical–thermal response arises from the interplay between MOF lattice softness, ion mobility, and light-activated interfacial processes.

By demonstrating self-cooling behaviour in a MOF-electrolyte hybrid, this work positions soft MOFs as active regulators of both energy and heat flow.[4] The results suggest a new design direction for energy storage materials in which framework flexibility, electrolyte chemistry, and photo-response are co-engineered to reduce thermal losses in continuously operating systems.By unifying light harvesting, energy storage, and thermal management within a single soft material, this approach points toward scalable strategies to reduce the resource and energy costs of future data and energy infrastructures.

Acknowledgement: KS acknowledges the financial support from The Leverhulme Trust through an Early Career fellowship ECF-2024-398 which has helped fund this work.

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IM - D3 - O13

Bifunctional luminescent Eu^{3+}-doped PMMA for building-integrated photovoltaics and visible-blind UV sensing

Irene Motta[1,2], Gregorio Bottaro[2,3], Maria Rando[1], Marzio Rancan[2,3], Lidia Armelao[1,3,4]
[1]Dept. of Chemical Sciences (DiSC), University of Padova, IT; [2] Institute of Condensed Matter Chemistry and Technologies for Energy (ICMATE), National Research Council (CNR), c/o Dept. of Chemical Sciences (DiSC), University of Padova, IT; [3]National Interuniversity Consortium of Materials Science and Technology (INSTM), IT; [3]Dept. of Chemical Sciences and Materials Technologies (DSCTM), National Research Council (CNR), IT

The luminescence properties of lanthanide complexes make them attractive to design multifunctional advanced materials, with applications spanning from laser materials to devices for energy harvesting and sensing.
In this work,[1] a family of Eu^{3+} bis-□-diketones has been used as dopant for poly(methyl methacrylate) (PMMA) to produce highly transparent, luminescent polymeric slates. These systems, exhibiting very high molar brightness, have been investigated first as Luminescent Solar Concentrators (LSCs) for building-integrated photovoltaics (BIPVs), with application as photovoltaic windows and as visible-blind UV photodetectors.
A series of PMMA/Eu^{3+} slates, 50 × 50 mm^2 wide and 3 mm thick, has been prepared by cast polymerization. The LSCs strictly absorb UV radiation, showing visual impact parameters comparable to those of window glass (AVT = 92%, CRI > 98, **Fig. 1**). They also show excellent UV-blocking properties, as they fully absorb AM1.5G radiation below 400 nm. Such wavelengths are known to be harmful to human health and to shorten the service lifetime of indoor furniture and flooring.
LSC-PV devices have been realized by coupling the PMMA/Eu^{3+} slates to Si solar cells. Electrical characterizations (J-V curves, EQE spectra) have been conducted in compliance with widely recognized guidelines for LSC reporting. The devices' performances replicate typical efficiencies of transparent LSC-PVs (**Fig. 2**). However, by employing super-bright luminophores, our systems show a most efficient use of europium, as they contain 10 to 100 times less Eu in weight with respect to analogous literature examples.
The characterization of the whole LSC-PV system for UV photodetection is also discussed. Considering the normalized detectivity D* as the figure of merit for sensitivity, the realized photodetectors exhibit performances comparable to best reported wide-band gap semiconductor heterojunctions, showing promising potential as large area, visible-blind photodetectors.

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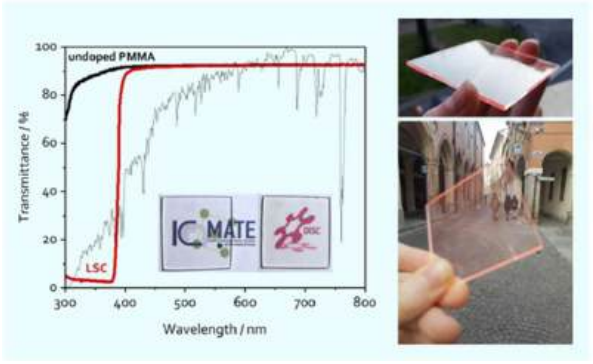

Fig. 3. Absorption spectra of the investigated LSC, demonstrating UV-blocking capabilities. Photographs of the LSC under daylight. The observed reddish color originates from the emission of Eu^{3+} complexes within the polymer matrix.

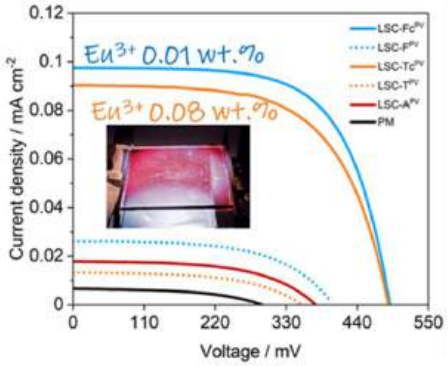

Fig. 2. Electrical output of the LSC-PV devices under 1 sun AM1.5G illumination. Optimized ligand design enables high performance with a reduced Eu^{3+} content.

IM - D3 - O15

Additively manufactured biomass-based 3D carbon frameworks as tunable supports for non-noble HER catalysts

Farnoosh Hormozinezhad[1], Laura Fuentes Rodríguez[1], Felipe A. Garcés Pineda*[2], Bahareh Khezri*[1,2,3]

[1]Dept. de Química Física i Inorgànica, Universitat Rovira i Virgili, ES; [2]Institute of Chemical Research of Catalonia (ICIQ-CERCA), The Barcelona Institute of Science and Technology (BIST), ES; [3]Catalan Institute for Research and Advanced Studies (ICREA), ES

Three-dimensional carbon architectures with engineered porosity can enhance electrochemical hydrogen evolution by improving mass transport, maximizing accessible surface area, and maintaining continuous electronic conduction. Yet producing such structures remains difficult because conventional carbon inks often offer limited printability and poor control over geometry. Here we introduce a polymer-templated additive-manufacturing strategy to fabricate micro-architected carbon scaffolds from lignin extracted from biomass feedstocks. In this approach, polymer lattices are first 3D printed to define the desired architecture, then impregnated with a lignin-based carbon precursor and calcined. During thermal processing, the polymer template is removed while lignin carbonizes, producing self-supporting 3D carbon frameworks that accurately reproduce the printed design.

This method decouples structural design from carbon processability, enabling tunable morphology, porosity, and connectivity without reformulating printable carbon materials. The resulting lignin-derived scaffolds provide interconnected pathways for electrolyte access, gas release, and electron transport, making them effective conductive supports for catalysis. To render the architecture, HER-active, the carbon frameworks are decorated with non-precious transition-metal catalysts (e.g., Ni, Cu, Fe, Mo, and bimetallic systems such as Ni/Cu and Ni/Fe), allowing catalyst chemistry and loading to be adjusted while preserving the 3D structure. With controllable architecture and adaptable catalytic interfaces, these materials offer a versatile platform for HER electrodes where efficient transport and bubble management are essential. Overall, this work establishes a sustainable route to advanced 3D carbon supports and underscores the promise of biomass-derived carbons for electrochemical energy technologies.

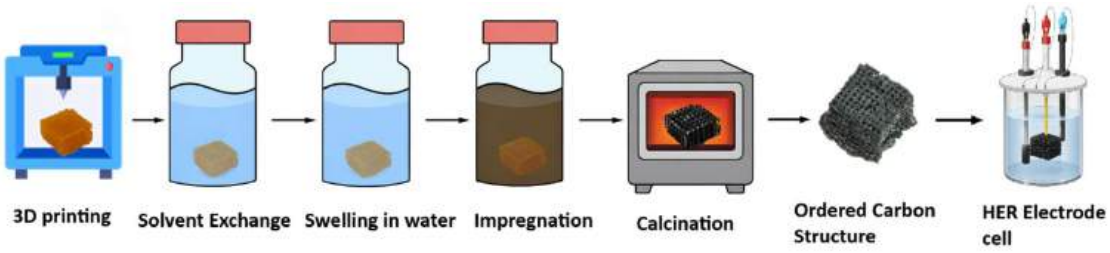

Fig. 1. Schematic illustration of the fabrication and application of an ordered carbon electrode. The process starts with 3D printing of the polymer scaffold, followed by solvent exchange (H_2O/DMF), swelling in water, and impregnation with lignin-based carbon precursors. Subsequent calcination converts the structure into an ordered carbon material, which is finally integrated as a working electrode in a HER electrochemical cell.

IM - D3 - O16

3D-printed photocatalytic reactors: Integrating stereolitography with hybrid TiO_2 materials

Isabel S.O. Barbosa[1], Yaidelin A. Manrique[1], Diana Paiva[2], Joaquim L. Faria[1], Ricardo J. Santos[1], Cláudia G. Silva[1]

[1]LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, PT; [2]LEPABE, ALiCE, Faculty of Engineering, University of Porto, PT

The integration of Additive Manufacturing (AM) with photocatalytic reactor design offers transformative opportunities for chemical synthesis and environmental remediation technologies. By enabling complex, tailored geometries, 3D-printed photoreactors can improve light distribution and catalyst exposure, thereby addressing core challenges in heterogeneous photocatalysis [1,2].

This work explores the fabrication and performance of 3D-printed photocatalytic structures produced via stereolithography (SLA), combining advanced manufacturing with catalyst immobilisation strategies. The reactor geometry (Fig.1) was designed to optimise internal light distribution, addressing a critical challenge in heterogeneous photocatalysis. A hybrid material was formulated by incorporating 1 wt% TiO_2 P25 Evonik, a benchmark photocatalyst, into a commercial photoreactive resin (Formlabs Clear V4), preserving printability while introducing functional photocatalytic properties. Comprehensive characterisation using scanning electron microscopy (SEM), rheology, and mechanical testing confirmed uniform dispersion of TiO_2 within the resin matrix and demonstrated that catalyst addition did not compromise the structural integrity or print resolution of the SLA-fabricated parts. Photocatalytic activity was evaluated through the degradation of Rhodamine B (RhB) as a model pollutant under controlled irradiation conditions.

The 3D-printed structures demonstrated robust performance, achieving significant RhB removal (Fig. 2), highlighting the potential of this fabrication approach for effective photocatalysis. Upon irradiation with 370 nm LEDs, an 80% decrease in RhB concentration was observed after 240 min. Whereas, in the absence of light, no RhB degradation occurred. Moreover, the photo-stability of the 3D structure was confirmed for at least 3 cycles of utilisation. Economic analysis further suggests that SLA-based production becomes cost-competitive in low to moderate volumes (≈7000 units), underscoring the viability of this strategy for scalable, customised reactor manufacturing.

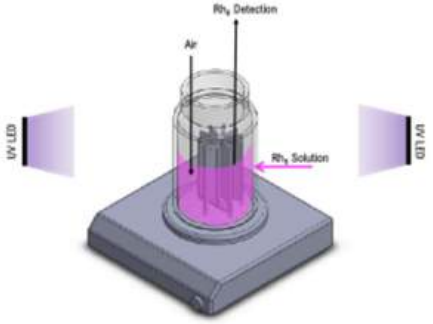

Fig. 1. Experimental setup of photocatalytic degradation of RhB.

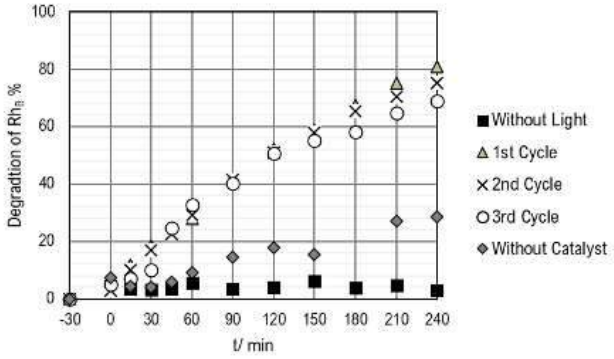

Fig. 2. Photocatalytic degradation of RhB over 3 consecutive cycles using Clear V4 + 1% TiO_2.

Overall, this study demonstrates a simple, rapid, and cost-effective route to produce photocatalytic reactors, bridging advanced manufacturing and environmental catalysis, with implications for water purification and sustainable chemical processing.

This work was financially supported by Fundação para a Ciência e a Tecnologia, I.P./MECI through national funds: LSRE-LCM, UID/50020/2025 (https://doi.org/10.54499/UID/50020/2025), and ALiCE, LA/P/0045/2020 (https://doi.org/10.54499/LA/P/0045/2020).

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IM - D3 - O17

Metal (oxo)clusters as photoinitiators: A direct route to covalently integrated PEGDA-hybrid hydrogels

Alina Petrovskaia[1], Stanislav Petrovskii[1], Eric Vogelsberg[1], Kirill Monakhov[1]
[1]Leibniz Institute of Surface Engineering (IOM), DE

Organo-functionalized Lindqvist-type $\{V_6O_{19}\}$-polyoxometalates (POMs) and octahedral $\{Mo_6X_8\}$-clusters represent two classes of inorganic building blocks, distinguished by their unique electronic architectures. The $\{V_6O_{19}\}$-based POMs are potent redox-active metal-oxo species capable of reversible or quasi-reversible multi-electron transfer and highly efficient charge delocalization.[1] In contrast, $\{Mo_6X_8\}$-clusters are robust, metal-metal bonded systems characterized by efficient phosphorescence and the ability to sensitize singlet oxygen via long-lived triplet excited states[2]. Both inorganic platforms offer exceptional modularity, allowing for extensive chemical tailoring through the modification of their surrounding ligand environments.
Integrating these responsive metal-organic units into polymer matrices is a proven strategy for developing high-performance functional materials. Traditionally, POM-polymer composites have been utilized to engineer high-performance proton exchange membranes,[3] as well as nanostructured redox-active electrodes for energy storage and biosensing.[4] Similarly, octahedral $\{Mo_6X_8\}$ cluster-based materials have emerged as promising, low-cytotoxicity candidates for both photodynamic[4] and radiodynamic[6] therapies.
In this work, we report a previously unexplored fundamental property of these metal (oxo)clusters: their capacity to serve as *photoinitiators for radical polymerization*. We leveraged this capability to synthesize a series of cross-linked PEGDA/cluster composites[7]. By employing a post-functionalization strategy, we developed a universal method for the covalent tethering of POM/cluster–organic hybrids bearing vinyl or acryl pendant groups. This approach ensures the robust immobilization of $\{V_6O_{19}\}$- and $\{Mo_6X_8\}$-cluster units within the copolymer matrix. Optimization of this technique led to the fabrication of elastic polymer films with high structural integrity, as application oriented biocompatible materials with potential antimicrobial properties.

Authors gratefully acknowledge funding by the DFG via project numbers 537270815 (House-of-Oxide) and 495326276 (PhotOcellMatrix).

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IM - D3 - O18
Harnessing the chemistry of two-dimensional materials

Stefano Ippolito[1], Paolo Samorì[2], Yury Gogotsi[3], Andres Castellanos-Gomez[1]
[1]2D Foundry Research Group, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), ES; [2]University of Strasbourg, CNRS, ISIS, FR; [3]A. J. Drexel Nanomaterials Institute, Dept. of Materials Science and Engineering, Drexel University, USA

All materials possess structural defects that strongly influence their physicochemical properties. This is particularly critical in two-dimensional (2D) materials, where defects behave as (re)active sites for functionalization reactions. Solution-processed semiconducting transition metal dichalcogenides (TMDs) are at the centre of an ever-increasing research in printed electronics, although the device performance still suffers from structural defects and poor inter-flake electronic connectivity. Recent and innovative defect engineering strategies use (di)thiolated molecules to heal sulfur vacancies via molecular chemistry approaches. In covalently interconnected TMD networks, the chemical structure of the dithiolated bridging linker is crucial and drastically influences the electrical device performance and charge transport mechanisms[1,2]. This strategy can also be applied to TMDs produced by various methods, including roll-to-roll exfoliation. Defects in solution-processed TMDs also favor toposelective reactions, leading to edge-decorated nanosheets with noble metal nanoparticles via galvanic displacement. Such mixed-dimensional materials show high performance in optical and photothermal sensing, electrocatalysis and electronics[3]. MXenes represent the latest and largest family of 2D materials. However, to leverage their potential in (opto)electronics, precise control over the chemical structure must be achieved. In Ti-based MXenes, the photothermal response strongly depends on their chemistry: Ti_2CT_x shows relaxation kinetics three orders of magnitude slower than $Ti_3C_2T_x$, improving thermal energy storage for tunable optical memory and neuromorphic applications[4].

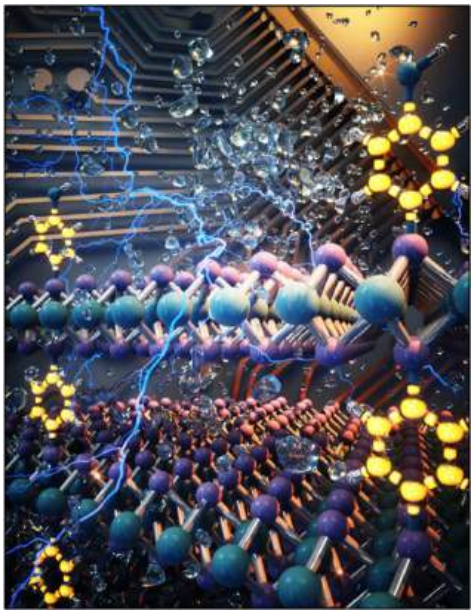

Fig. 1. Illustration showing covalently interconnected MoS_2 networks obtained by using π-conjugated dithiolated molecules, which exhibit superior performance in electronic devices.

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IM - D3 - O19

Turning PVC waste into value: upcycled PVC-based single-chain nanoparticles for catalytic applications

José A. Pomposo[1,2,3]

[1]Materials Physics Center (CFM-MPC), ES; [2]University of the Basque Country (UPV/EHU), ES; [3]IKERBASQUE-Basque Foundation for Science, ES

This presentation introduces an innovative and complementary strategy for the valorization of polymer waste through the upcycling of a widely used commodity plastic—polyvinyl chloride (PVC).[1] Our approach enables the direct transformation of PVC into functional, "valorized" single-chain nanoparticles (SCNPs) providing a molecular metamorphosis pathway that converts an abundant, low-value waste material into high-performance macromolecular nanostructures.[2]

The full upcycling process is carried out in *N*-butylpyrrolidone , a dipolar aprotic solvent considered a greener alternative to more hazardous solvents commonly used for PVC processing. When precipitation or purification steps are required, a simple ethanol/water mixture serves as an effective non-solvent. This methodology yields well-defined, uniform PVC single-chain nanoparticles that exhibit excellent stability in the solid state, maintaining their structural integrity for several months without degradation.

A particularly remarkable aspect of this system arises when 7.3 mol% of Cu(II) ions is incorporated into the PVC-SCNPs. This modification generates highly efficient and recyclable nanocatalysts for the solvent-free homocoupling of polar alkynes, showing significant activity under mild conditions. Furthermore, the Cu-functionalized PVC-SCNPs display enzyme-mimetic catalytic behavior, efficiently promoting the oxidation of 3,5-di-*tert*-butylcatechol to its corresponding *o*-quinone.[3] In addition, they demonstrate exceptionally high turnover frequency, TOF, in the peroxidative oxidation of styrene to benzaldehyde, highlighting their versatility and potential relevance in both academic catalysis research and industrially oriented oxidation processes.

Revalorizing post-consumer PVC waste by converting it into sustainable, robust catalytic nanomaterials offers a conceptually powerful example of how end-of-life plastics can be transformed into new functional materials.

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IM - D3 - F01
From 1D to 2D: On-surface synthesis of conjugated polydiacetylene monolayers

Jie Zhang[1], Sven Bernaerts[1], Aurelio Mateo-Alonso[2], Kunal S. Mali[1], Steven De Feyter[1]
[1]Division of Molecular Imaging and Photonics, Department of Chemistry, KU Leuven, BE; [2]POLYMAT, University of the Basque Country UPV/EHU, ES

On-surface synthesis, a bottom-up fabrication strategy, enables the controlled conversion of preorganized diacetylene (DA) derivatives into structurally defined polydiacetylene (PDA) films via thermally or photochemically initiated radical polymerization.[1–3] These conductive polymers have shown applications in optoelectronics and colorimetric sensors.[4-6] Yet obtaining long-range ordered 2D PDAs remains challenging, because topochemical 1,4-addition is strongly geometry-dependent and typically yields isolated 1D chains. In this contribution, we present an experimental protocol based on 2,5-(10,12-henicosadiynyloxy) terephthalic acid (TTA-DIA) that self-assembles on graphite into an interdigitated molecular network. Upon UV irradiation the reactive monolayer stitches laterally into a covalently integrated 2D PDA. High-resolution STM/AFM provide real-space evidence of 2D covalent connectivity and resolve the structural details. A process map identifies an operating window in heptanoic acid with an optimum exposure of 30 min, yielding near-uniform coverage over 2 × 2 μm² imaging area and polymer domains up to 1-2 μm². The growth mode is atmosphere-dependent: air enables 2D propagation, whereas N_2/Ar favors 1D growth and produces sparse TTA-DIA polymers. We also observe ordered self-folded stacking of lifted backbones. To our knowledge, this establishes **the first large-area, laterally covalent two-dimensional polydiacetylene monolayer with micrometer-scale order on substrate** and provides a reproducible platform and mechanistic basis for device-ready conjugated architectures.

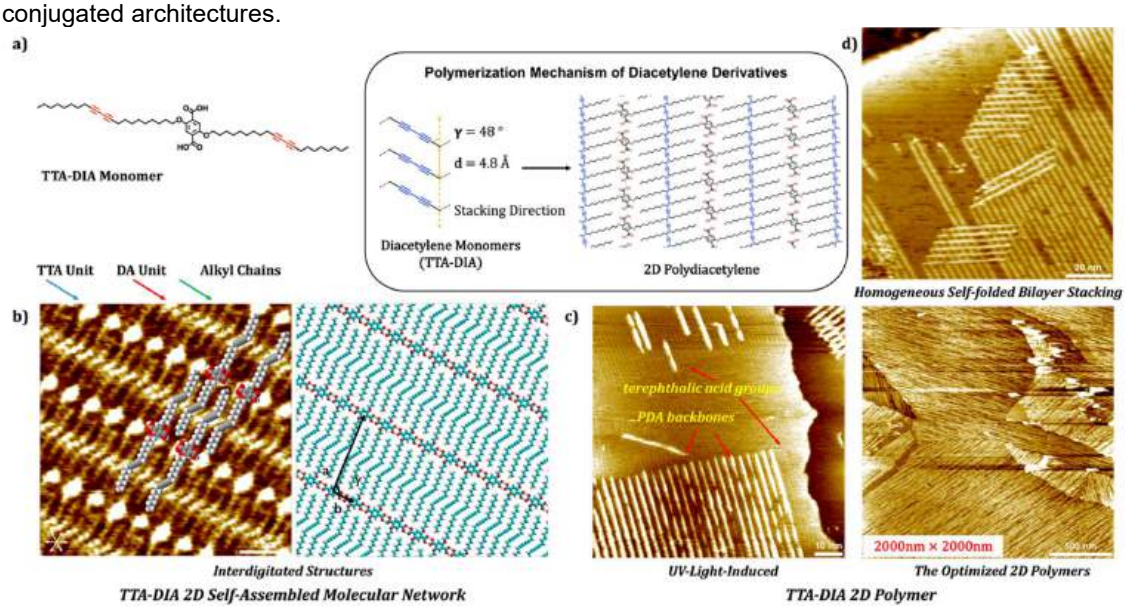

Fig. 1. (a) Chemical structures of TTA-DIA and schematic of the topochemical polymerization that yields the TTA-DIA 2D polymer. (b) High-resolution STM image of the two-dimensional self-assembled molecular network of TTA-DIA with the corresponding structural model. (c) STM images showing UV-induced 2D polydiacetylene network on HOPG, including a representative optimized-yield state. (d) STM images of a self-folded bilayer of the TTA-DIA 2D polymer.

Acknowledgements: This work is supported by the European Union under the Horizon Europe grant 101046231 (FantastiCOF) and by M-ERA.NET (SuperSuper) call via FWO project G0K9822N. KU Leuven–Internal Funds (C14/19/079) is acknowledged.

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IM - D3 - F02

Beware of the structure: Insights into the phosphorus dynamics of post-synthetically modified NU1000 in the presence of water

J. Theissen[1,2], E. Derveaux[2], R. Narvaez[3], S. Smeets[2], N. Gys[1], F. Tielens[3], P. Adriaensens[2], W. Marchal*[2], R. Ameloot*[1]

[1]Centre for Membrane Separations, Adsorption, Catalysis, and Spectroscopy (cMACS), KU Leuven, BE; [2]Institute for Materials Research (IMO-IMOMEC), Analytical and Circular Chemistry (ACC), UHasselt, BE; [3]General Chemistry (ALGC) - Materials Modelling Group, Vrije Universiteit Brussel, BE

Understanding the structure and chemistry of materials at the atomic scale is essential to elucidate and rationalize their properties as a key step to boost their application in future technologies. Metal-organic frameworks (MOFs) are porous coordination polymers formed by the ensemble of metal ions or clusters and organic linkers, offering a large versatility and tunability in surface area, chemical composition, and thermal stability. These properties are attractive for various applications, including gas storage and separation, catalysis and sensing [1]. These applications can be explored by introducing new chemical entities into the MOF framework by metal node functionalization via solvent-assisted ligand incorporation (SALI) [2]. In this study, we investigate the post-synthesis modification of the Zr_6 metal node in NU-1000 MOF by reaction with phenylphosphonic acid (PhPA), yielding the material NU-1000-PhPA (Figure 1, A).

To probe the dynamic behaviour of this modified material in response to water, the material was stored under different storage conditions, and we performed solid-state ^{31}P-MAS NMR (Figure 1B) and two-dimensional dipolar heteronuclear correlation (^{1}H-^{31}P HETCOR) experiments (Figure 1C). ^{31}P-MAS experiments provided valuable insight into the local phosphorus environment, enabling a detailed analysis of the structural evolution under different hydration conditions. DFT simulations confirm the presence of chemisorbed PhPA and their difference in chemical shift as a function of humidity. It allowed us to distinguish between different phosphorus coordination modes and regions within the MOF where water and hydrogen bonding is either present or absent, depending on the loading of PhPA.

This study highlights the advantages of 2D dipolar HETCOR NMR techniques in elucidating the structural changes and coordination environments within MOFs, providing deeper insights into the role of water in modulating material properties over time.

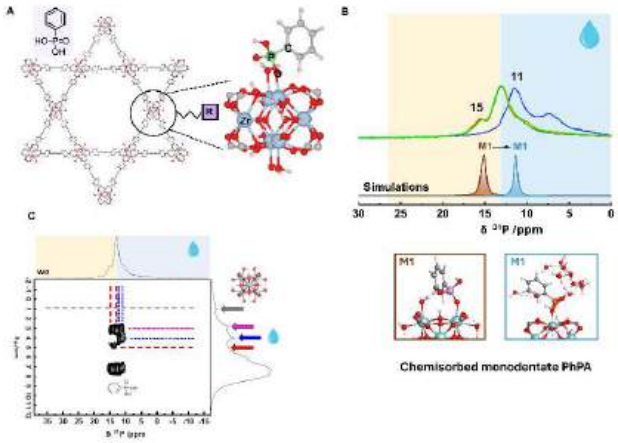

Fig. 2. (A) Post-synthetic modification of the Zr_6 metal node in NU-1000 MOF. (B) ^{31}P-MAS NMR of dry NU-1000-PhPA (green), water-exposed NU-1000-PhPA (dark blue) and the DFT simulations, enabling to distinguish the chemical environment in correlation with water. (C) ^{1}H-^{31}P HETCOR NMR of NU-1000-PhPA.

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IM - D3 - F03

Bio-based polymeric films for the photocatalytic degradation of contaminants of emerging concern in aqueous media

Michela Tramontini[1], Meagan Mehlhop[1 3], Rossella Sesia[2], Marco Sangermano[2], Paola Calza[1]
[1]University of Turin, IT; [2]Polytechnic of Turin, IT; [3]University of the Basque Country, ES

The growing occurrence of emerging contaminants in aquatic environments is a major environmental concern, particularly pharmaceuticals, whose toxicity, persistence, and resistance to conventional treatment technologies are poorly understood. These limitations highlight the need for sustainable and effective remediation strategies.

In this study, bio-based polymeric films derived from epoxidized linseed oil (an abundant and potentially biodegradable vegetable oil) were prepared via UV-curing and evaluated for the removal of contaminants of emerging concern from water, using diclofenac as a model molecule. The films acted as multifunctional supports for an indium P-doped graphitic carbon nitride (In_1-P_5 g-C_3N_4) photocatalyst, iron (II/III) chlorides, and horseradish peroxidase, enabling the combination of photocatalytic, Fenton-like, and enzymatic degradation processes. Single- and dual-layer film architectures were developed to integrate multiple degradation mechanisms within a single polymeric network. Photocatalytic performance was strongly dependent on catalyst loading, with films containing 1.9% In_1-P_5 g-C_3N_4 achieving complete diclofenac degradation within two hours and a pseudo-first-order rate constant of 0.054 ± 0.005 min^{-1}. The combined adsorption-photodegradation approach proved most effective and was successfully applied to diclofenac removal in real water matrices, spanning from river water to aquaculture water.

The photodegradation pathways of diclofenac were assessed as well via HPLC-MS and three main transformation products were identified, whose toxicity was assessed using *in silico* structure–activity relationships. While two by-products were predicted to be more toxic than the parent compound, their concentrations decreased significantly over time, whereas the most abundant product was considerably less toxic. Overall, these hybrid, vegetable oil-based films represent a promising, eco-friendly platform for the remediation of pharmaceutical contaminants in water.

Acknowledgements: This work was funded by the European Union's Horizon 2020 Research and Innovation Programme under the MSCA Grant Agreement No101007578 (SusWater).

IM - D3 - F04

Engineering nanoscale amorphous calcium phosphate through molecular and polymeric stabilization strategies

Debora Briganti[1], Rita Gelli[1], Francesca Ridi[1]
[1]*Dept. of Chemistry "Ugo Schiff" and CSGI, University of Florence, IT*

Amorphous calcium phosphate (ACP) combines strong bio-relevance with remarkable chemical versatility, making it an appealing building block to engineer nanoscale carriers and responsive platforms[1]. ACP use, however, is still limited by intrinsic instability: in aqueous media ACP readily aggregates and progressively converts into crystalline phases, compromising dispersibility and hampering the key advantages of the amorphous state. To address this bottleneck, we developed a molecular and polymeric stabilization route to engineer ACP-based nanometric particles by acting directly on nucleation and early growth, where size and phase evolution are determined. Molecular or polymeric stabilizers enable fine control over both colloidal behaviour and amorphous-phase persistence. In this framework, bisphosphonates bind calcium species in solution and interact with the forming calcium phosphate clusters, regulating growth pathways and shifting the resulting particle size distributions. Beyond size control, this systematic study shows that colloidal stability can be tuned as a function of bisphosphonate chain length, identifying molecular architecture as a practical design parameter. Polyacrylate provides a complementary strategy by strongly limiting irreversible clustering and yielding ACP-based dispersions with excellent redispersibility upon handling and storage[2]. Particle dimensions can be further adjusted through composition: varying magnesium content offers an additional, independent strategy to regulate the size of the obtained particles. To link stabilizer chemistry to particle properties, the systems were investigated through a multi-technique workflow, combining dynamic light scattering (size in suspension), electron microscopy (morphology), X-ray diffraction together with IR spectroscopy (phase/crystallinity), and thermal analysis (amorphous-to-crystalline conversion). Overall, these results outline a simple and experimentally grounded approach to obtain ACP-based sub-micron particles with tunable size and controllable stability, supporting their development as formulation-ready platforms for nanomedicine.

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IM - D4 - O01

Interface-engineered MoS_2 photo-nanozymes as multifunctional materials for precision catalytic cancer therapy

Almudena Marti[1], Alida Monjovelo[1], Filippo Pieretti[1], Arthur Reymond[1], Robert Wojcieszak[1], Amandine Szczesnowski[2,3], Henri-Pierre Lassalle[2,3]

[1]L2CM, CNRS, University of Lorraine, UMR 7053, Vandoeuvre-lès-Nancy, FR; [2]Institution Université de Lorraine, CNRS UMR 7039, CRAN, Nancy, FR , [3]Institut de Cancérologie de Lorraine Nancy, FR

Tumor hypoxia and limited therapeutic efficacy present significant challenges in cancer therapy.[1] Catalytic nanomaterials, particularly photo-nanozymes, have emerged as innovative materials to address these limitations through the integration of catalytic and photophysical functions. By combining peroxidase (POD), catalase (CAT), and oxidase-like (OXD) activities with near-infrared (NIR) activation, photo-nanozymes enhance reactive oxygen species (ROS) generation, alleviate hypoxia, and enable localized photothermal heating, offering a multifunctional platform for precision catalytic cancer therapy.[2]

Herein, we report interface-engineered MoS_2-based photo-nanozymes as advanced multifunctional materials. Hydrothermally synthesized MoS_2 nanoflowers (~200 nm) exhibit intrinsic POD- and CAT-like activities, efficiently converting endogenous hydrogen peroxide into ROS and oxygen, directly mitigating tumor hypoxia.[3] C_3N_4@MoS_2 heterojunctions were engineered to enable tunable optical absorption, improved charge separation, and cascade catalytic activity. Varying MoS_2 content (5–40 wt%) allowed precise control of NIR-induced temperature rise ($\Delta T \approx 10$ °C, 808 nm). In vitro studies using 2D FaDu cells and 3D tumor spheroids showed minimal dark toxicity and potent photothermal/ROS-mediated cytotoxicity. The synergistic integration of cascade catalysis, oxygen generation, ROS amplification, and localized photothermal heating enables fine-tuned tumor microenvironment control[4], transforming hypoxia from a therapeutic barrier into a targetable feature. Interface engineering further enhances multifunctionality, tunability, and catalytic performance.

Overall, MoS_2-based photo-nanozymes constitute a robust, interface-engineered multifunctional platform for precision catalytic cancer therapy. By uniting enzymatic mimicry with photothermal functionality, this work highlights the potential of photo-nanozymes as next-generation materials for advanced oncology applications.

This project received financial support from the CNRS through the MITI interdisciplinary programs and from Lorraine Université d'Excellence as part of the FR 2030 Program (reference ANR-15-IDEX-04-LUE). This communication is based on the work from COST Action LUCES (CA22131).

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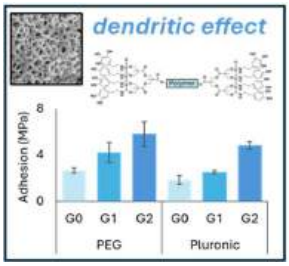
IM - D4 - O02
Multidentate catechol-functionalized biomimetic dendrimers: Self-assembly and adhesion

Alexandre Lancelot[1,2], Jonathan Wilker[2], Teresa Sierra[1]
[1]Instituto de Nanociencia y Materiales de Aragón - CSIC, ES, [2]Purdue University, USA

Catechol moieties are found in several proteins secreted by mussels and other bivalves, allowing them to firmly adhere to sea reefs. Such catechol moieties can foster strong adhesive interactions through H-bonding, π-π stacking, metal chelation and covalent bonding.[1] Accordingly, by mimicking mussels' proteins, a library of biomimetic catechol-containing polymers has been synthesized as new versatile adhesives.[2]
In the present work,[3] two series of Linear-Dendritic Block Copolymers (LDBCs) were synthesized. They contain: *(i)* a linear polyether polymer, either poly(ethylene glycol) *(PEG-LDBC series)* or poly(ethylene glycol)-poly(propylene glycol)-poly(ethylene glycol) *(Pluronic-LDBC series)*, *(ii)* 2,2-bis(hydroxymethyl) propionic acid dendritic blocks of generation 0, 1 and 2, and *(iii)* terminal catechol moieties. When used as bulk adhesives, both PEG-LDBC and Pluronic-LDBC series exhibited strong adhesion when applied to aluminium substrates, with adhesion values of up to 7 MPa. Moreover, the dendritic architecture demonstrated its relevance for adhesion, as multidentate adhesives showed higher adhesion values, thereby linking molecular design to material performance.
Additionally, the Pluronic-LDBC series self-assembled in water, forming first micelles and subsequently hydrogels, depending on concentration and temperature. CryoSEM observations revealed that different hydrogel pore sizes were obtained as a function of dendritic generation. All hydrogels showed adhesive properties, being able to glue porcine skin in *ex vivo* assays with adhesion values up to 3 kPa, paving the way for potential future biomedical applications of these materials.



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IM - D4 - O03

Brominated tyrosines: From pathology biomarkers to the design of resilient and strain-stiffening peptide-based materials

Elisa Marelli[1], Claudia Pigliacelli[1], Lorenza Draghi[2], Chiara Russo[3], Monica Soncini[3], Pierangelo Metrangolo[1]
[1]Laboratory of Supramolecular and Bio-Nanomaterials, and [2]Before Lab, Dept. of Chemistry, Materials, and Chemical Engineering "Giulio Natta", [3]Biomolecular Engineering Lab, Dept. Electronics, Information and Bioengineering, Politecnico di Milano, IT

Resilin, an elastomeric protein found in arthropods, possesses remarkable mechanical properties such as high resilience and elasticity, making it an attractive candidate for bioinspired materials. However, translating these unique properties in synthetic materials has remained a challenge, primarily due to the protein's intricate structure and extensive amino acid sequence.[1] In our recent work, we focused on the modification of the resilin consensus sequence SDSYGAP through bromination of the tyrosine residue.[2] This minimal alteration induced peptide self-assembly due to the increased supramolecular stability conferred by bromine atoms,[3,4] resulting in a robust three-dimensional network of fibrils within a hydrogel matrix, which exhibited elastic properties absent in the wild-type sequence. Building upon these findings, this study explores the combination of this modified peptide with other biomaterials, such as gelatin, and the fabrication of nanofibrous mats through electrospinning. This technique offers precise control over scaffold morphology and architecture, enabling tunable mechanical properties and excellent biocompatibility. We successfully produced electrospun nanofibers having uniform morphology, and showing strain-stiffening behaviour and recovery properties characteristic of biological tissues, highlighting the potential of the fabricated scaffolds for various biomedical applications.[5] Furthermore, the brominated heptapeptide scaffolds demonstrated antioxidant activity and enhanced proteolytic stability, attributed to the inherent properties of the peptide sequence. This study promises the development of biomimetic materials with tunable mechanical properties and added functionalities, inspired by Nature's design.

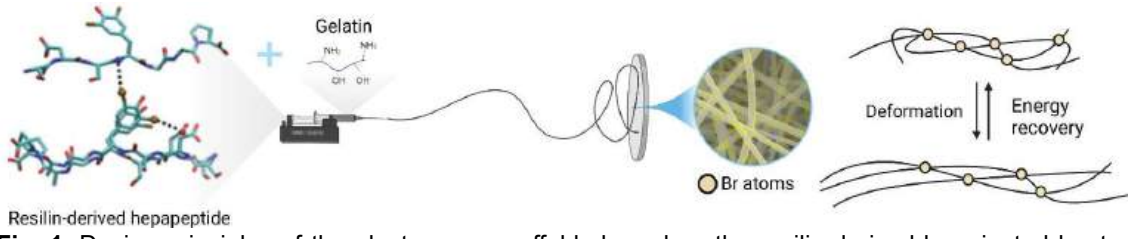

Fig. 1. Design principles of the electrospun scaffolds based on the resilin-derived brominated heptapeptide combined with gelatin.

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IM - D4 - O04
From laboratory to reality: Surface engineering by hydrogel transfer printing

Shubham Tiwari[1,4], Alejandra Arias Peña[1], Markus Biesalski[2], Oswald Prucker[1], Luisa Goldmann[3], Jan Lübke[3], Gottfried Martin[3], Günther Schlunck[3], and Jürgen Rühe[1,4]
[1]Dept. of Microsystem Engineering (IMTEK), Albert Ludwigs Universität Freiburg, DE; [2]Macromolecular Chemistry and Paper Chemistry, Technical University of Darmstadt, DE; [3]Eye Center, Medical Center − University of Freiburg, Faculty of Medicine, University of Freiburg, DE; [4]Cluster of Excellence livMatS @ FIT–Freiburg Center of Interactive Materials and Bioinspired Technologies, Albert Ludwigs Universität Freiburg, DE

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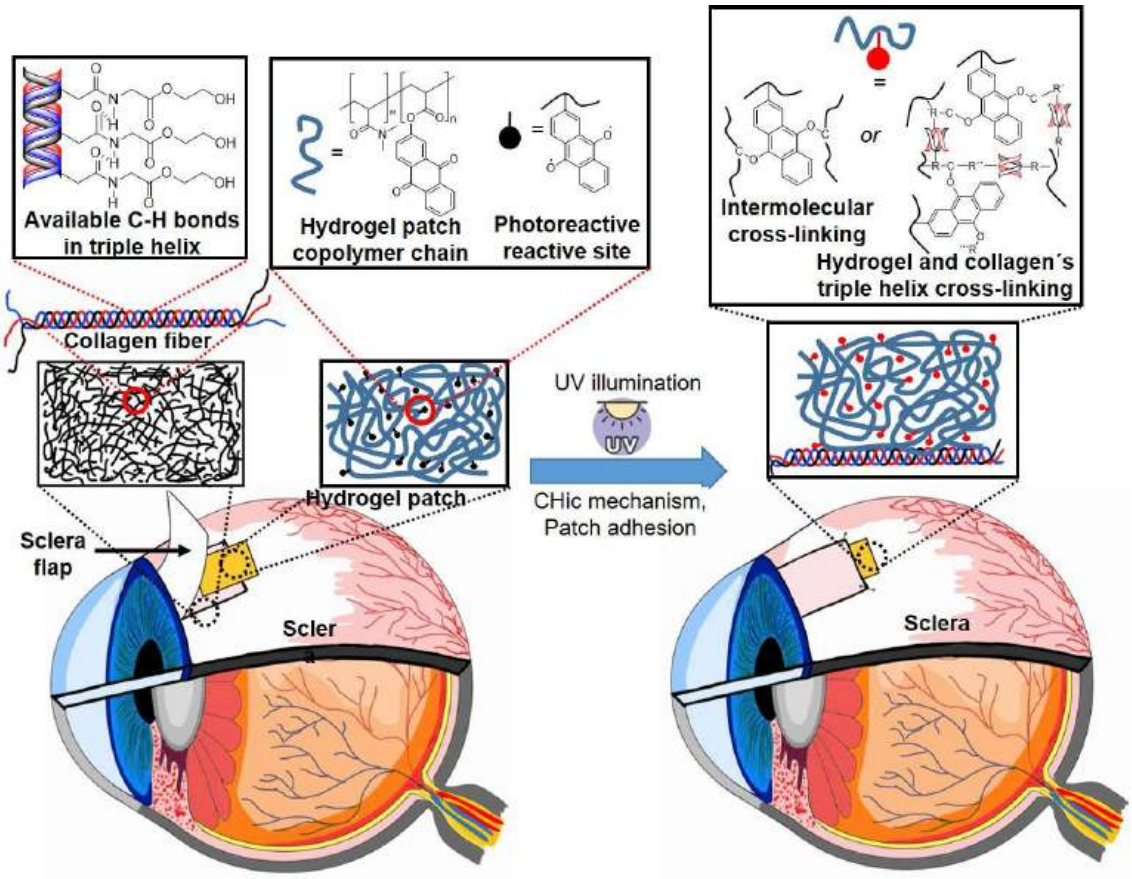

Coating materials with hydrogel layers is important for the performance of many modern biomedical materials, but it often proves difficult on substrates with complex, non-planar topologies. Additionally, achieving permanent adhesion to the substrate can be challenging, particularly when water is present, as it causes the hydrogel to swell. We introduce a hydrogel transfer printing technique that uses special paper as a substrate and a C-H insertion reaction. The paper acts as a flexible transfer agent and has a controlled hydrophobic and a hydrophilic side. A photoreactive hydrogel precursor is deposited on its hydrophobic side, which is then placed on the target surface. Adding a small amount of water to the hydrophilic side releases the hydrogel precursor and enables smooth transfer to the desired substrate. After removing the transfer paper, brief UV illumination activates the deposited photopolymer, leading to crosslinking and covalent attachment of the layer to the substrate surface via CHic.
An emerging advancement in glaucoma, a leading cause of blindness, has been achieved by transfer printing, which demands innovative and effective treatments that surpass the limitations of current drug and surgical interventions to lower intraocular pressure. This approach employs cell-repellent patches deposited via transfer printing, composed of a hydrophilic, protein-repellent prepolymer hydrogel based on a copolymer of dimethylacrylamide and a comonomer bearing anthraquinone moieties. Upon transferring the hydrogel patch to the desired location, brief irradiation with UV light with the wavelength of 365 nm simultaneously induces crosslinking and covalent attachment to the ocular surface via C–H insertion reactions, resulting in robust and stable integration.

We also demonstrate the handling and attachment of these hydrogels to substrates with varying, complex topologies along with cellulose and biological, with brief UV irradiation which allows the deposition of hydrogel layers with high accuracy and uniformity, as well as excellent underwater adhesion.

Acknowledgements: Carina Breuer (TU Darmstadt) is thanked for her helpful advice on the paper and Luisa Goldmann for the cell experiments at University clinic. The authors are grateful to Marcel Eckert for the development of the copolymer. Natalia Schatz is thanked for the copolymer synthesis and Daniela Mössner for polymer characterization, Yi Thomann from livMatS for SEM imaging. This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under the projects DFG-Sklera: RU489/27-3 (Sklera III, 2100356701) and Zeiss IPROM: 2100210801. Additional support from the Cluster of Excellence Living, Adaptive, and Energy-autonomous Materials Systems (livMatS), EXC-2193/1-390951807, is gratefully acknowledged.

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IM - D4 - O05

Efficient Immobilization and recovery of the C–H bond-activating LsAA9A on functionalized mesoporous silica

F. Careddu[1,2], C. Pontremoli[1], Kelsi R. Hall[3,4], M. Sørlie[3], V. G. H. Eijsink[3], C. Barolo[1], S. Bordiga[1]
[1]University of Torino, Torino, IT; [2]University School for Advanced Studies IUSS Pavia, IT; [3]Norwegian University of Life Sciences, Ås, NO; [4]University of Canterbury, NZ

Lytic polysaccharide monooxygenases (LPMOs) are mononuclear copper-dependent enzymes that catalyze the oxidative cleavage of glycosidic bonds in recalcitrant polysaccharides, making them promising catalysts for oxidative biotransformations. However, their industrial application is limited by high susceptibility to oxidative inactivation, particularly under substrate-free conditions[1,2]. Active site confinement is crucial for LPMO functionality and stability, in native systems, the substrate itself provides a docking surface that shields the exposed copper site. Immobilization on solid supports therefore represents an effective strategy to enhance enzyme stability, provided that the approach is simple, cost-effective, and preserves activity.
In this study, the engineered LPMO LsAA9A from *Lentinus similis* was covalently immobilized onto amino-functionalized mesoporous silica nanoparticles. This support was selected based on previous immobilization studies on carbon nanotubes, where increased dispersion of CNT–LPMO systems hindered catalyst recovery[3]. SBA-15-type NH_2-functionalized silica was synthesized via a sol–gel method and characterized by infrared spectroscopy, thermogravimetric analysis, and scanning electron microscopy, confirming a well-defined mesoporous structure with the desired surface functionality. The NH_2/SBA-15 materials were activated with glutaraldehyde and used for LsAA9A immobilization by targeting surface-exposed lysine residues, thereby promoting active site confinement.
The immobilized enzyme retained both oxidase and peroxygenase activities toward small oligosaccharides such as cellopentaose (Gluc5), yielding product conversions comparable to the free LPMO, while enabling efficient catalyst recovery and reuse for up to six oxidative cycles.
Overall, these results highlight that rational support design is essential not only for preserving LPMO catalytic performance but also for practical aspects such as separability and recyclability, paving the way toward durable and sustainable LPMO-based biocatalysts.

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IM - D4 - O06

Enhanced stability and reusability of recombinant silicatein upon biomimetic metal–organic framework crystallization

Tongtong Zhang[1,2], Xiangyu Wang[1], Jack D. Wright[1], George F.S. Whitehead[1], Jeremiah P. Tidey[3], Lu Shin Wong[2], Imogen A. Riddell[1]

[1]Dept. of Chemistry, The University of Manchester, UK; [2]Manchester Institute of Biotechnology, University of Manchester, UK; [3]Dept. of Physics, University of Warwick, UK

Performing selective chemical transformations under benign and environmentally friendly conditions – as achieved in nature by enzymes - is a key goal in industrial chemistry. Biocatalysis offers an attractive, and sustainable, alternative to traditional chemical processes but has not had the widespread industrial uptake that was initially anticipated due to the poor stability of many enzymes outside of their natural environment. In this work we demonstrate, for the first time, the power of MOF biomimetic crystallisation for the stabilisation of inherently unstable enzymes. In our enzyme@MOF composites the MOF controls the microenvironment around the enzyme constraining its movement, thus offering a generalisable methodology which achieves the goal of stabilization without requiring modification to the enzyme

Specifically, we focus on the immobilisation of silicatein within an appropriately chosen protective MOF.[1] Silicatein is an established but elusive biotechnological target which catalyses the metathesis of Si-O bonds under ambient conditions offering the prospect of a greener route to synthesise silicones. Current routes to Si-O bond-forming reactions, employed extensively in the synthesis of siloxanes and silyl ethers, present environmental and safety challenges. To date, development of an enzymatic approach to Si-O bond transformations has eluded scientists due to the lack of stability of silicatein, resulting in poor recyclability. Here, we demonstrate that biomimetic crystallization provides a route to a MOF-silicatein composite that is stable in aqueous and organic solvents, and can be reused over multiple reaction cycles. We also demonstrate that immobilisation of silicatein within an appropriately chosen MOF extends the enzyme half-life at room temperature from days for the native enzyme to months for the encapsulated enzyme. Biomimetic MOF crystallization thus represents a robust approach to the stabilization of biocatalysts for process intensification.

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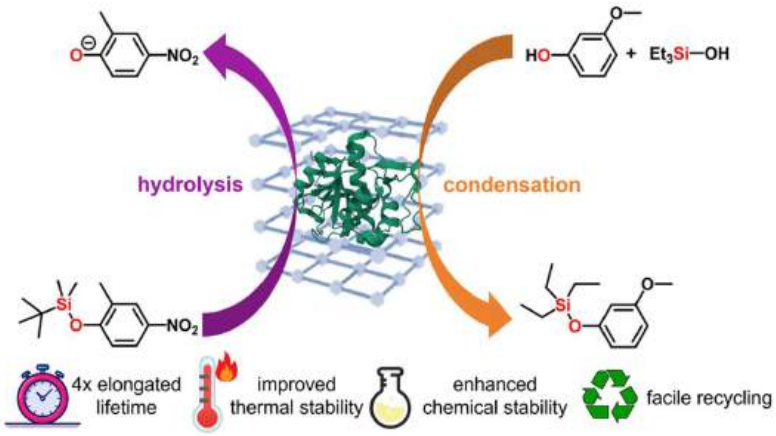

Fig. 1. Schematic depicting silicatein@MOF and the Si-O hydrolysis and condensation reactions evaluated in this study. MOF immobilisation increases the lifetime of silicatein at room temperature, improves the enzymes thermal and chemical stability and enables its recycling.

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IM - D4 - O07

Rheology-guided development of polymeric microneedles for controlled delivery of pembrolizumab in triple-negative breast cancer

Anna Palma[1], Elena Lagreca[1], Fabrizia Rossi[1], Giuliana Allocco[1], Sara Coppola[2], Daniele Tammaro[1], Pier Luca Maffettone[1], Concetta Di Natale[1]

[1]University of Naples Federico II, Dipto di Ingegneria Chimica, dei Materiali e della Produzione Industriale, IT;
[2]Institute of Applied Sciences and Intelligent Systems (ISASI), National Research Council of IT (CNR), IT

The development of advanced polymeric materials requires precise control over formulation and processing to achieve localized and controlled delivery of biologics. Here, we present a rheology-guided materials design approach for the fabrication of dissolvable polymeric microneedles (MNs) incorporating biodegradable microparticles (MPs) loaded with pembrolizumab, developed as a model immune checkpoint inhibitor for localized delivery applications [1].

Microneedle arrays were manufactured using an advanced pyro-electrohydrodynamic (p-EHD) process, which relies on pyroelectric-induced deformation of polymer droplets into high-aspect-ratio microstructures [2]. To address key challenges in formulation processability and structural reproducibility, precursor materials were systematically optimized by correlating bulk rheological properties (viscosity, shear-thinning behavior, and flow response) with interfacial parameters, including surface tension [3]. This combined rheological interfacial tuning enabled stable droplet deformation under the pyroelectric field, uniform MP incorporation, and preservation of antibody integrity during fabrication.

The optimized MN materials exhibited favorable shear-responsive behavior, mechanical robustness compatible with pain-free application, and controlled degradation profiles. In vitro release studies demonstrated an initial burst followed by sustained pembrolizumab release while maintaining structural and functional stability. Functional validation using patient-derived triple-negative breast cancer tumor organoids confirmed effective localized delivery, enhanced tissue penetration, and activation of immune related response pathways.

Overall, this work demonstrates how rational control of rheological and interfacial properties can enable the scalable fabrication of advanced polymeric microneedle materials using p-EHD technology. The proposed strategy provides a versatile materials-driven framework for the development of next-generation platforms for localized and controlled delivery of biologics.

Acknowledgment: FIS-2023-01644 PINCH “Polyvalent mIcroNeedles in triple breast Cancer fight”- CUP E53C25000410001 - MUR FONDO ITALIANO PER LA SCIENZA 2022 – 2023.

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IM - D4 - O09
Functional hydrogel microstructures: Design, fabrication and stimulus-induced actuation

Annael Sort-Montenegro, Jason Delente, Žiga Roblek, Yekaterina Tskhe, Colm Delaney, Larisa Florea
School of Chemistry & AMBER, The SFI Research Centre for Advanced Materials and BioEngineering Research, Trinity College Dublin, IE

Stimuli-responsive hydrogels have the ability to undergo volume changes in response to stimuli such as temperature, light, magnetic and electric fields, or chemistry of the local environment. My group's research focuses on the development of responsive polymers and hydrogels that can switch between different states upon exposure to external stimuli. Micro-fabrication of these materials using direct laser writing (DLW) by two-photon polymerisation (2PP) provides a suitable route for the 3D fabrication of micro-actuators and sensors showing fast, reversible and tailored response.
By merging the advantages of 2PP-enabled micro-fabrication with stimuli-responsive polymers, we demonstrate the realisation of sophisticated 3D micro-structures that can possess features associated with biological systems, in particular the ability to switch or change characteristics in response to desired stimuli. Furthermore, fine control of mechanical properties can be achieved in 3D through programmed control of laser parameters (laser power, writing speed, slice and hatching distance), to achieve structures which can undergo anisotropic and programmable shape change upon stimulation (i.e. 4D response). This is achieved by combination of the 3D design process, and prediction of the real-time response, using Finite Element Analysis (FEA).
During this talk I will give several illustrations of 3D micro-structures based on hydrogels and hydrophilic polymers, that can respond to external stimulation, actuate on demand, and sense and report on their local chemical environment.[1,2] One such example is shown in Figure 1, where electro-actuator microstructures based on copolymers of gelatin were micro-fabricated via 2PP (Figure 1A), to produce both anionic and cationic polymer networks capable of sustaining electro-actuation (Figure 1B&C) displaying fast response (200 ms) and large equilibrium bending angles of up to 44.9 ± 7.8° (Figure 1D). Such responsive microstructures have applications in medical devices and soft micro-robotics.

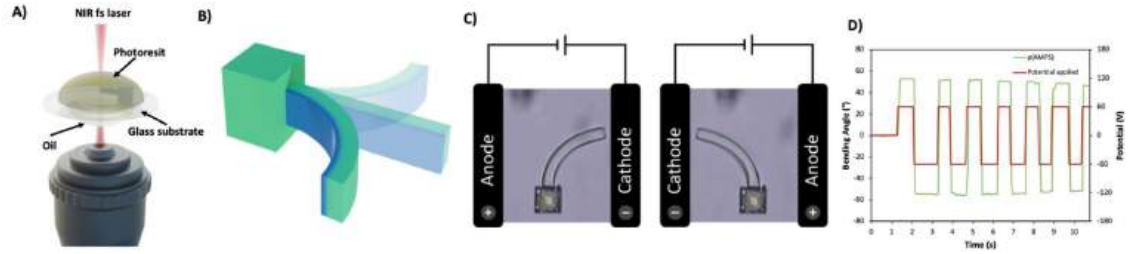

Fig. 1. A) Micro-fabrication setup based on multi-photon polymerisation for the fabrication of micro- actuators; **B)** Schematic representation of the micro-cantilever actuation upon applying an electric stimulus to the electrolyte solution; **C)** Microscope images of micro-cantilevers fabricated by DLW, upon application of an electric potential of 60 V and reversing the polarity; **D)** Bending angle of a micro-cantilever (80 × 10 × 20 μm^3) upon the application of an electric field of 6 $V \cdot mm^{-1}$.

This research received funding from the European Research Council (ERC) Starting Grant (No. 802929 - ChemLife), and Research Ireland under the SFI Frontiers for the Future Programme (22/FFP-P/11541) and 12/RC/2278_P2. J.D. acknowledges support from Research Ireland through GOIPD/2022/550 and the European Horizon 2020 Research and Innovation Programme (no. 899349 – 5D NanoPrinting).

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IM - D4 - O10

Two-photon lithography as enabling technology for the fabrication of conformal electrodes on 3D microstructures and devices

Marco Carlotti[1,2]

[1]Dipt. di Chimica e Chimica Industriale, University of Pisa, IT; [2]Center for Materials Interfaces, Istituto Italiano di Tecnologia, IT

Direct laser writing (DLW) is an innovative technology based on two-photon polymerization processes, which allows the 3D printing of architectures with arbitrary complexity at the (sub)micrometer scale. As such, this platform is becoming increasingly appealing for the fabrication of soft microsystems, MEMS, metamaterials, and functional surfaces.

While most of the research interest in this field relies on additive manufacturing, subtractive approaches can be extremely helpful in nano/microfabrication of complex devices, allowing the preparation of expendable scaffolds, replaceable parts, and protection for fragile structures.

In this study, different strategies are proposed to enable the fabrication of high-quality conformable electrodes on complex 3D microstructures using DWL-printed 3D conformable sacrificial masks and innovative designs. In particular, these include the addition of cyclic ketene acetal compounds to different acrylate-based photoresists, resulting in versatile functional formulations that allow the 3D-printing of degradable poly(ester-co-acrylate) microstructures via DLW.[1] These latter could be degraded reliably under mild conditions compatible with other photoresists and materials of common use in the fabrication of MEMS, thus opening new opportunities to design novel fabrication procedures.

In addition, new designs were investigated that allowed the preparation via DLW of 3D-conformal shadow masks which can be removed by mechanical means, thus not requiring any chemical removal step, which might interfere with delicate functional materials often employed in the preparation of responsive soft microdevices.

Finally, these approaches are employed for the direct fabrication of organic electrochemical transistors on complex, non-flat, non-horizontal 3D structures, thereby demonstrating the capabilities of these methodologies in the realization of functional devices that combine complex architectures and on-board signal processing with micrometric and submicrometric resolution.

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IM - D4 - O11

Understanding plasma polymerization using complex geometry substrates: A step toward the design of gradient nanostructures

Robin Dantinne[1], Philippe Leclere[2], Claude Poleunis[3], Arnaud Delcorte[3], Damien Thiry[1]
[1]Chimie des Interactions Plasma-Surface (ChIPS), CIRMAP, University of Mons, BE; [2]Laboratory for Physics of Nanomaterials and Energy (LPNE), CIRMAP, University of Mons, BE; [3]Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain (UCL), BE

Plasma polymerization has become a well-established method for synthesizing organic thin films known as plasma polymer films (PPF). However, the underlying growth mechanism remains only partly understood, notably due to the limited methods available for probing microscopic processes occurring at the growing film interface. Nevertheless, recent works have shown that plasma polymerization on substrates with complex geometries, such as “cavities” and “undercuts”, could provide a deeper insight into the surface growth mechanism of PPF.[1]

In this context, this work furthers this approach by investigating the influence of dissipated power and substrate temperature on three-dimensional plasma polymerization, two synthesis parameters well-known to influence plasma processes on planar substrates. Allyl-alcohol is used as a model precursor for plasma polymerization on undercut substrates.

XPS measurements reveal a significant decrease in oxygen content (up to 6%) as the coating reaches deeper into the undercut structure. Similarly, ToF-SIMS indicates a decrease in cross-linking degree compared to films deposited on planar substrates. These changes correlate with an evolution of the glass transition temperature as evaluated by ToF-SIMS experiments and are explained by the uneven diffusion of various reactive species as well as the limited ionic bombardment in undercut substrates resulting in gradient PPF properties. In contrast, the viscoelastic behavior of PPF is found to be similar for 3D- and 2D-deposited coatings, ranging from rigid solid to viscous liquid depending on the synthesis conditions.

Additionally, the uneven deposition profile on 3D substrates allows for the determination of the surface loss probability (β) of the film-forming species, revealing a decrease in β with Ts.

Finally, an innovative approach taking advantage of the inhomogeneous properties of 3D-deposited PPF and the wrinkling phenomenon is developed for the fabrication of nanowrinkled metallic surfaces with gradient nanostructure dimensions, of interest for various applications in optics, catalysis and biotechnology (see Figure 1).

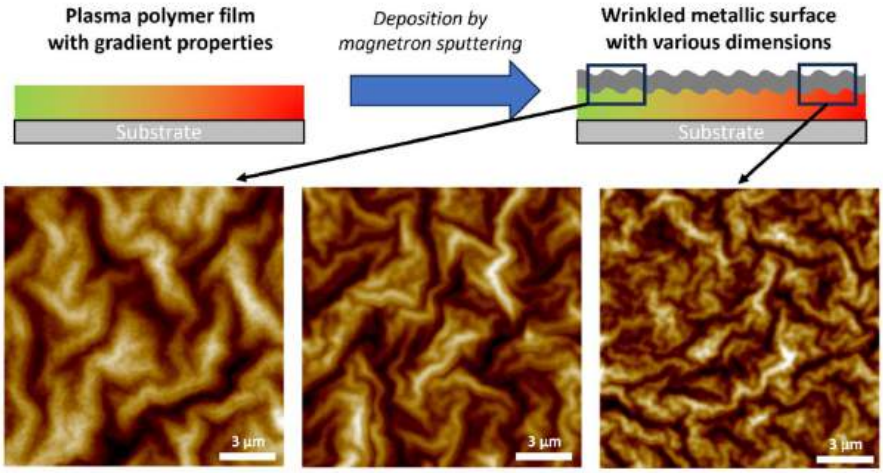

Figure 1. Schematic representation of the wrinkling process applied on plasma polymer films with gradient properties. A bilayer system made of a bottom viscous PPF and a top stiff metallic layer will spontaneaously give rise to wrinkles. The wrinkle dimensions evolve with the properties of the bottom layer, yielding gradient nanostructures.

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This work is supported by the French Community of BE within the framework of a FRIA grant.

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IM - D4 - O12

PDMS-based nano- and microstructures for tailoring optical properties across the hyperspectral range

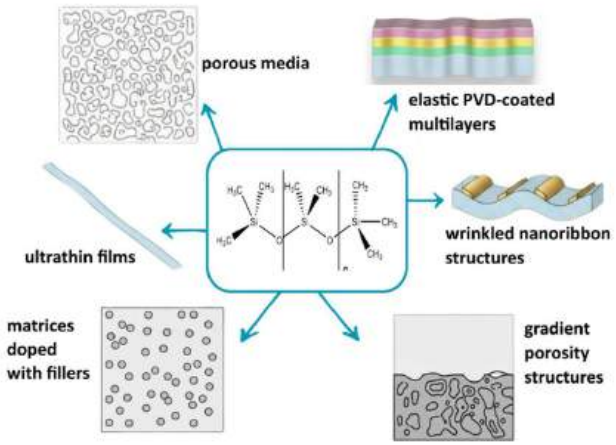
Patrycja Wytrych, Urszula Malecka, Patrycja Barańczyk, Weronika Bielecka, Alexander Korneluk, Tomasz Stefaniuk

University of Warsaw, PL

Polydimethylsiloxane (PDMS) is an organosilicon elastomer built from a Si–O–Si backbone with methyl side groups, which jointly determine its key physicochemical properties. Chemically, PDMS is largely inert and resistant to many aqueous and mild chemical environments, while its low surface energy and crosslinkable network enable straightforward replication and integration with coatings or functional inclusions. Mechanically, it combines a low elastic modulus with high elasticity, allowing conformal contact to textured surfaces and reversible deformation—features that are especially valuable when optical functionality must be tuned by strain or shape change. Optically, PDMS is highly transparent throughout most of the visible spectrum and remains usable into the infrared, where molecular vibrational bands introduce wavelength-selective absorption that can either limit transmission or be exploited for spectral shaping. These combined attributes make PDMS an attractive base material for reconfigurable nano- and microstructures with a mechanically tunable optical response.

We systematically evaluate various PDMS-based architectures to determine which configurations provide superior hyperspectral control over effective refractive index and scattering, and consequently define the material's reflectance and emissivity. Furthermore, we identify structures exhibiting the strongest mechano-optical modulation under tensile strain. Our comparison encompasses: (i) surface-engineered systems such as PVD-coated multilayers and wrinkled nanoribbon structures; (ii) volumetric composites incorporating fillers like ground PDMS powder, polyethylene, TiO_2, or SiO_2; and (iii) porous media featuring controlled voids and gradient porosity. We detail fabrication protocols and link processing–structure relationships to hyperspectral performance, offering design guidelines for strain-tunable PDMS photonics across the VIS–IR range.

The versatility of these architectures opens new avenues for devices operating across the electromagnetic spectrum. For example, passive radiative cooling emerges as a promising direction, leveraging the optimized infrared emissivity and durability for efficient thermal management. Beyond thermal control, these concepts can also inspire broadband light-management coatings and strain-tunable, mechanically reconfigurable optical components.



IM - D4 - F02

Molybdenum sulfide - Chitosan hydrogels as model platforms for the delivery of antibody-drug conjugates

María Gutiérrez-Blanco[1,2], Sébastien Harlepp,[2] Loïc Charbonniere[1], Alexandre Detappe[1,2*]
[1]Institut Pluridisciplinaire Hubert Curien, CNRS/Université de Strasbourg, FR; [2]Institut Strauss, FR

Metal-polymer hydrogels typically combine either natural (e.g., chitosan, alginate, hyaluronic acid) or synthetic matrices (PEG, PAA, polyacrylamides) with mono- or divalent metal ions as cross-linkers.[1] In such systems, the nature and coordination chemistry of metal components play a central role in defining network architecture and macroscopic properties. This class of hydrogels have been investigated as drug depots for delivery of small molecules and proteins. However, they have not yet been employed for the delivery of next-generation therapeutics.

Among targeted therapies, antibody drug conjugates (ADCs) represent a promising tool as they offer outstanding activity and selectivity in cancer treatment.[2] ADCs are composed of a cytotoxic drug (payload) linked to an antibody through a chemical linker. While intravenous (IV) administration remains the main delivery route for these biomacromolecules, subcutaneous (SC) administration is emerging as a powerful alternative improving the pharmacokinetics and the patient's life quality through a less invasive strategy.[3]

We thus developed a new ADC delivery platform based on metal-polymer hydrogels containing an unprecedented cross-linking motif (i.e., trinuclear Mo_3S_4 clusters)[4] that generated chitosan gels under physiological conditions compatible with SC administration (Figure 1). This model system was used to gain insights into the release mechanism of several ADCs, and their dependence on macroscopic and microscopic properties of both the gel and drugs. We foresee that our results will help to fine-tune the upcoming systems to obtain a controlled and sustained delivery.

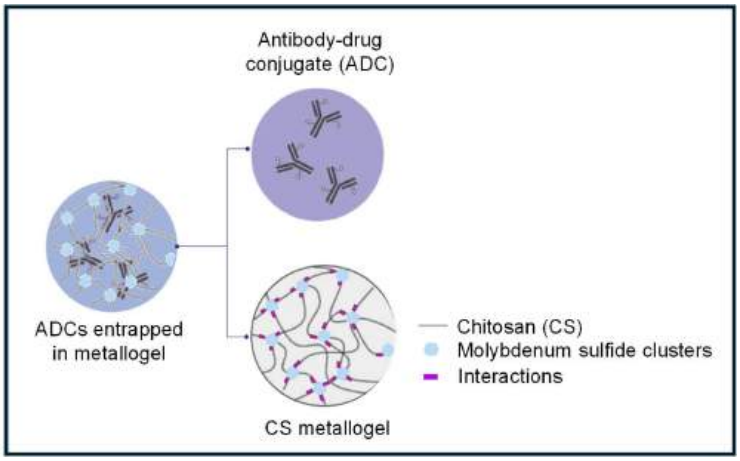


Fig. 1. Schematic representation of the metal-chitosan hydrogel used as a model platform for ADC delivery

This work was supported by the European Research Council (ERC) Starting Grant TheranoImmuno, grant agreement No. 95010, the Institut de Cancérologie Strasbourg Europe and Gustave Roussy Foundation. This project has also received funding from the Fondation pour la Recherche Medicale through a postdoctoral fellowship (SPF202409019620)

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IM - D4 - F04

Electrospun TiO_2/BiOI heterostructured nanofibers for solar-driven water decontamination

Laura Huidobro[1,2], Mahmoud Abid[3], Mikhael Bechelany[3], Elvira Gómez[1,2], Albert Serrà[1,2]
[1]Dept. de Ciència de Materials i Química Física, Universitat de Barcelona, ES; [2]institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, ES; [3]Institut Européen des Membranes (IEM), University of Montpellier, FR

The design and development of photocatalytic nanomaterials is key to addressing the increasing difficulty of eliminating persistent and emerging pollutants from aquatic environments. In this study, networks of TiO_2 nanofibers were produced through electrospinning and subsequently modified with BiOI using a solvothermal procedure performed for different reaction times, which enabled the creation of TiO_2/BiOI heterostructures.
To evaluate their performance, the materials were tested in the degradation and mineralization of sulfamethoxazole (SMX) as well as in multipollutant water mixtures under both visible and UV irradiation. The transformation routes of SMX were examined by identifying intermediate compounds via HPLC, offering insight into the reaction mechanisms. Mineralization, that is, the complete conversion of pollutants into CO_2 and water, was evaluated by total organic carbon (TOC) measurements. The role of peroxymonosulfate (PMS) was also investigated, showing that it enhances mineralization due to its photoactivation and the subsequent formation of sulfate radicals capable of oxidize organic matter. In addition, the potential of these photocatalysts to promote microplastic degradation was assessed. The long-term chemical stability of the heterostructures was analyzed through ICP measurements to detect photocorrosion, alongside reusability tests that confirmed their stability after repeated cycles. Results obtained from multipollutant samples further demonstrated the broad applicability of the system. Finally, ecotoxicity assays were performed to ensure that the treated water did not exhibit harmful effects, confirming the environmental compatibility of the process.
Electrospun TiO_2/BiOI nanofibers show strong chemical robustness, photocatalytic activity under visible light, and high versatility, positioning them as promising candidates for solar-driven water purification technologies.

Acknowledgements: The authors would like to express their gratitude to the Dept. de Recerca i Universitats, particularly the Dept. d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR) for their support.

IM - D4 - F05

Uncovering synthesis-structure-function relationships in $ZnFe_2O_4$@TiO_2 Z-scheme photocatalysts

Samar Al Jitan[1], Pegie Cool[1], Sofie Cambré[1], Sabine van Doorslaer[1], Vera Meynen[1]
[1]*University of Antwerp, BE*

Photo(electro)catalytic (PEC) CO_2 conversion is a promising route for using renewable energy to mitigate climate change[1], but its efficiency is limited by rapid recombination of photo-generated charge carriers, especially under low bias[2]. Direct Z-scheme heterojunctions can overcome this limitation by enhancing charge separation and extending charge-carrier lifetimes[3]. This project aims to improve CO_2 photo(electro)conversion efficiency by understanding how $ZnFe_2O_4$ morphology and the extent of $ZnFe_2O_4$/TiO_2 interfacial contact influence Z-scheme performance in catalytic powders.

As a foundation for this work, we conducted a systematic study to optimize the wet-chemical synthesis of $ZnFe_2O_4$, a key component of the proposed heterojunctions. We found that several understudied parameters, notably filtration method, solution aging, crucible covering, and pre-calcination grinding, substantially influence precursor purity, nucleation behavior, crystallinity, and crystallite size. For example, centrifuge filtration yielded more homogeneous precursors and smaller crystallites, while aged solutions altered nucleation pathways and final crystal structure. Thermogravimetric analysis further showed that optimized samples exhibited minimal mass loss and negligible thermal transitions.

Building on these insights, $ZnFe_2O_4$@TiO_2 nanocomposite powders with varied $ZnFe_2O_4$ morphologies and TiO_2:$ZnFe_2O_4$ ratios are being synthesized and then characterized by XRD, Raman, FTIR, diffuse reflectance spectroscopy, SEM-EDS, and XPS. Their photocatalytic performance toward CO_2 reduction is also being evaluated. This work provides new understanding of $ZnFe_2O_4$ synthesis control and its impact on Z-scheme heterojunction formation.

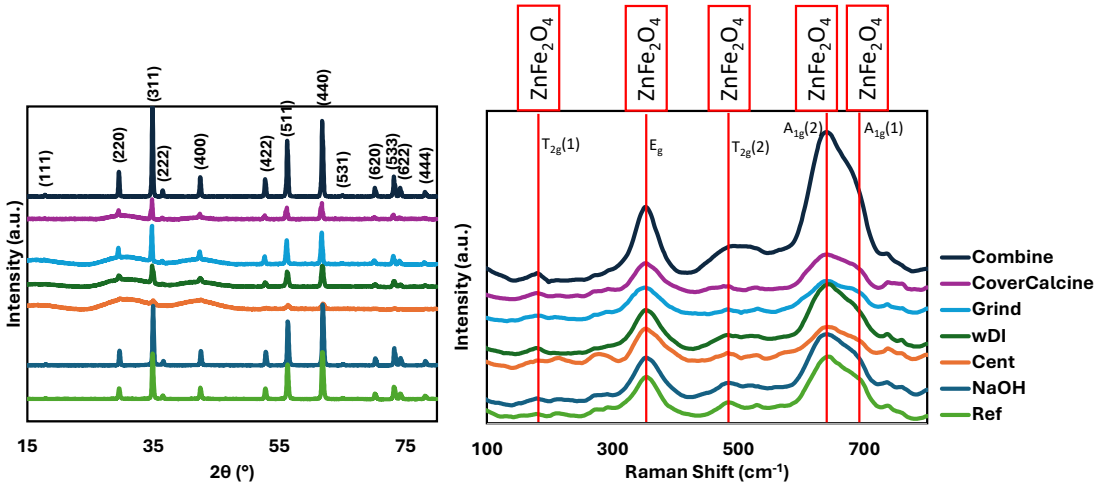

Fig. 1. (Left) XRD patterns and (Right) Raman bands of $ZnFe_2O_4$

This work has received financial support from the European Research Executive Agency under the action HORIZON TMA MSCA Postdoctoral Fellowships - European Fellowships, project 101204943 - PROSCOPY.

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Molecular Design & Reactivity (MDR)

MDR - D1 - O01

Thiophene functionalized hexavanadate hybrids: Modular synthesis and studies of their adsorption on Au(111) surfaces and gold nanoparticles

Stanislav K. Petrovskii[1], Marco Moors[1], Alina Petrovskaia[1], Ahmed Alsadig[2], Larysa Baraban[2,3], Kirill Monakhov[1]

[1]Leibniz Institute of Surface Engineering (IOM), Germany; [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany; [3]Dresden University of Technology (TUD), Germany

Immobilization of functional molecules on surface interfaces is a key fundamental objective on the way from the discovery of chemico-physical properties to their implementation into real-world molecular-based electronics and hybrid composite materials prototypes.[1] Redox activity and switching characteristics of hexavanadates supported by tris-alkoxo ligands and the general robustness of this class of polyoxometalates (POMs) make them very attractive objects of research with far-reaching goals for the development of extremely efficient electronic devices.[2]

Chemisorption on technologically relevant gold interfaces generally implies an introduction of sulfur-bearing fragments. However, the strongly oxidative behavior of Lindqvist hexavanadates poses a challenge for the installation of reductive S(II) centers, especially highly reactive thiolate –SH functionalities. A feasible alternative is the installation of thiophene pendant groups that combine the higher stability of an aromatic structure with the substrate-specific immobilization on Au surfaces.[3]

In the the current study, a series of V_6-thiophene covalent conjugates (Fig. 1) was synthetized by exploiting the modular 'click' chemistry post-functionalization.

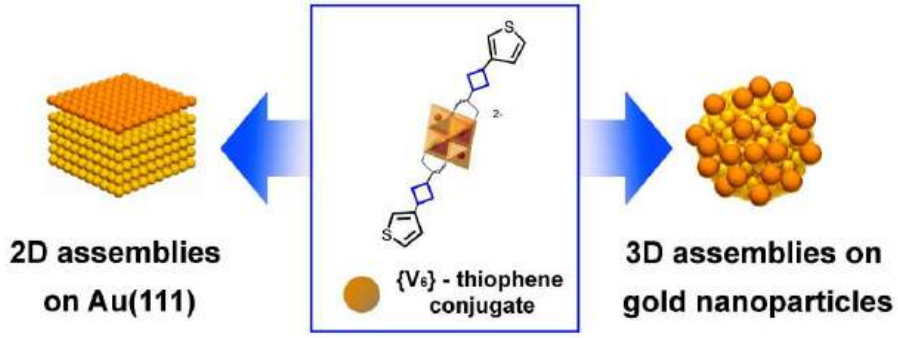

Fig. 1. Formation of 2D and 3D assemblies on gold interfaces by the adsorption of thiophene-functionalized V_6 hybrids.

The molecular hybrids obtained were examined towards adsorption on Au(111) and gold nanoparticles (AuNPs). Comprehensive studies by means of physical methods has revealed the nanoscale organization and adsorption behavior of V_6 species on 2D and 3D interfaces and confirmed their efficient surface immobilization on gold interfaces.

As a result, a bottom-up strategy, including modular synthesis and molecular design of inorgano-organic hybrids bearing switchable V_6-cores and their immobilization on technologically relevant gold interfaces, was developed.

The Authors gratefully acknowledge funding by the DFG via project numbers 558671949 (CovPOMNet) and 495326276 (PhotOcellMatrix).

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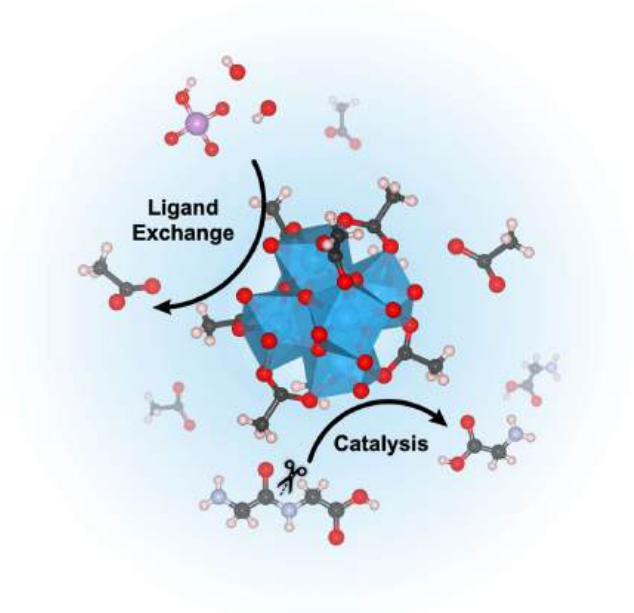
MDR - D1 - O02

Ligand exchange in Zr/Hf-Oxo clusters: Mechanistic insights and implications for catalysis

Kilian Declerck[1], Nada D. Savic[1], Muhammed J. Parammal[2], Carlotta Seno[2], Jonathan De Roo[2], Tatjana N. Parac-Vogt[1]

[1]KU Leuven, Belgium; [2]University of Basel, Switzerland

Atomically precise group IV metal-oxo clusters, consisting of structured Zr/Hf oxo nodes capped by exchangeable ligands, are rapidly emerging as versatile catalysts at the interface of homogeneous and heterogeneous chemistry. Their activity stems from the inherent Lewis acidity and oxophilicity associated with the metal centers, enabling coordination to electron-donating functional groups like carboxylates, phosphates, and amides. By controlling the accessibility of the Lewis acidic sites via the identity, number, and mobility of surface ligands, we precisely tuned the oxo cluster reactivity toward amide bond hydrolysis in peptides and proteins. This reaction serves as an ideal benchmark because substrate activation requires direct interaction with the metal-oxo cluster. Unlike extended solid catalysts, such as metal-organic frameworks and bulk metal oxides, discrete oxo clusters undergo rapid ligand exchange at their surfaces, which in turn governs substrate binding, activation, and product release. Another advantage of Zr/Hf-oxo clusters is their tunable solubility which enables their use as catalysts under either homogeneous or heterogeneous conditions. Using a combination of soluble and insoluble Zr/Hf-oxo clusters, our work demonstrated that the ligand dynamics critically modulate reactivity in solution and at solid-liquid interfaces. We specifically (i) examined the soluble Zr_6 cluster, where ligand exchange drives activity[1], (ii) investigated the insoluble Zr_{17} cluster, where the ligand shell modulates reactivity by influencing adsorption/desorption dynamics[2], and (iii) performed a comparative study of soluble and insoluble Hf_{12} clusters[3], highlighting how ligand shell occupation controls reactivity. Together, these studies underscore a unifying principle: control over ligand exchange at cluster surfaces provides a powerful handle for tuning catalytic activity. By directly linking the ligand shell chemistry to reactivity, we aim to provide a roadmap for designing next-generation cluster catalysts with enhanced stability, selectivity, and recyclability.



Ligand exchange is a central paradigm underlying metal-oxo cluster catalysis.

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MDR - D1 - O03
Charged pathways in bent-core design: Pyridine scaffolds for next-generation soft materials

Aleksandra Mašulović, M. Blanca Ros
Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, Spain

Liquid crystals (LCs), offering the uniqueness of structural order and fluidity, have played a pivotal role in low-energy display technologies, driving progress in portable electronics. Their self-organizing nature provides anisotropic optical, electrical, mechanical, and magnetic properties that can respond to external stimuli[1]. Looking for heterocyclic-based LC designs, pyridine stands out as a particularly versatile central scaffold not only altering the electronic properties but also imparting a dipole moment, which can strongly influence mesophase behavior[2]. Moreover, simple protonation of the pyridine rings provides straightforward access to ionic LCs, affording amphiphilic self-assembly in solution and lamellar ordering in the solid state[3]. In parallel, supramolecular design strategies have revealed that covalently tethering a cation and anion within the same molecule creates zwitterionic systems with unique physicochemical behavior that supported by non-covalent interactions and self-organizational tendencies, offer enhanced opportunities for constructing nanostructured, functional soft materials. Together, neutral, ionic, and zwitterionic pyridine-based motifs provide a rich and highly tunable platform for engineering advanced liquid-crystalline systems[4,5].
We present synthesis and characterization of two systematic series of bent-core molecules based on pyridine cores. Within each series, neutral derivatives, their corresponding cationic analogues and zwitterionic forms were synthesized. In parallel, tetraethylene glycol (TEG)-substituted derivatives were prepared in both neutral and cationic forms for each backbone. All compounds were fully characterized by NMR, MS and EA and their liquid-crystalline properties were investigated using polarized optical microscopy and differential scanning calorimetry, demonstrating that both series of bent-core systems exhibit rich mesomorphic behavior strongly dependent on molecular charge state and terminal chain functionality. In addition to bulk mesophases, selected compounds were processed into supramolecular aggregates, organogels and thin films, highlighting their potential as versatile soft materials. This study demonstrates how controlled structural variation within bent-core pyridine systems enables fine tuning of LC properties and material processability.

Acknowledgments: This work is part of the BCLC-TANGO project [GA101153257] funded by the Marie Skłodowska-Curie Actions (MSCA), Horizon Europe Programme (2021-2027), and the Gobierno de Aragón research group project E47_23R.

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MDR - D1 - O04
Structure-dependent antimicrobial activity of polyoxometalate-polypeptide hybrid materials

Paula Novella-Rodríguez[1], Rafael Martín-Rapún[1,2], Scott G. Mitchell[1,2]
[1]Institute of Nanoscience and Materials of Aragon(INMA), CSIC-University of Zaragoza, Spain; [2]CIBER de Bioingeniería, Biomateriales y Nanomedicina, Instituto de Salud Carlos III, Spain

Biofilms are structured bacterial communities embedded in an extracellular polymeric matrix that protects them from harsh conditions, enabling uninterrupted growth and differentiation that promotes resistance to conventional antibiotics. Because these resistant microorganisms pose a serious risk to human health, new antimicrobial strategies are needed to prevent biofilm formation and combat antimicrobial resistance.
In our team, we have explored the covalent conjugation of polyoxometalates (POMs) and antimicrobial polypeptides to benefit from the synergic effects that arise from the combination of both components. [1]In these studies, anionic POMs were functionalised with small organic molecules which act as linkers, facilitating the conjugation of synthetic antimicrobial polypeptides. [2]Crucially, the peptidic portion of the corresponding hybrid material combines cationic and non-polar residues which interact and disrupt bacterial cell membranes. Our work has shown that redox activity of the POM and the self-assebly of the hybrids are key to their biological activity against model bacteria strains. [3] Here I will illustrate how synthetic modifications to the peptide architecture influence the chemical properties of the polypeptides, which translates to a change in the biological activity of the corresponding hybrid materials. Recent results have shown how changing the peptide architecture while maintaining similar global compositions of the POM-peptide hybrid has an effect on the antibacterial activity of our materials. Self-assembly studies are being conducted with our latest materials, and further compositions are being explored to expand our library of POM-peptide hybrid materials.

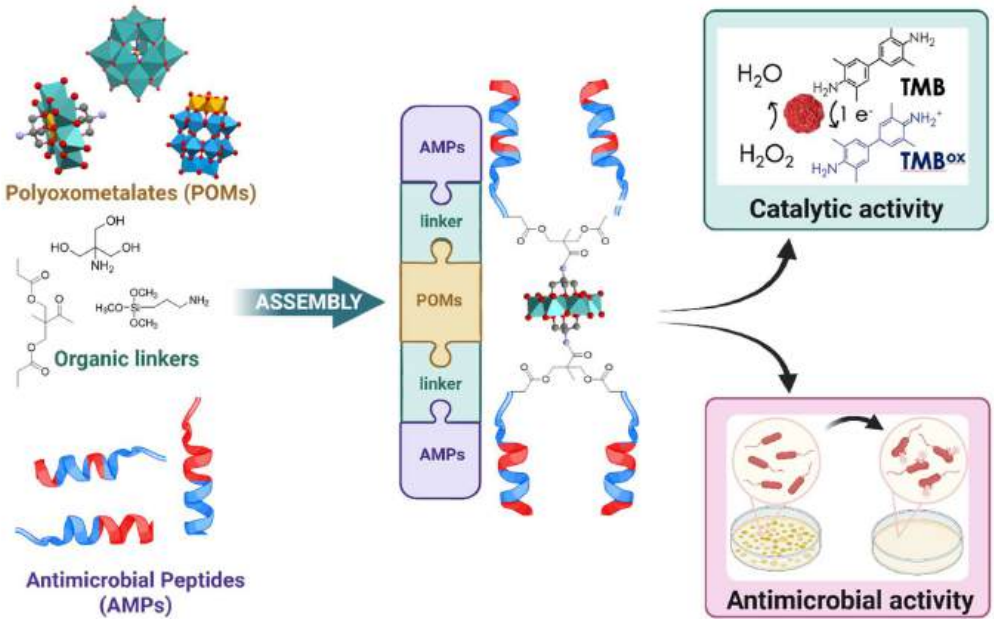

Fig. 1. Overview of the development of POM-peptide hybrids.

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MDR - D1 - O05

Polyoxometalate-based metal-organic assemblies towards supramolecular catalysis and functional materials

Cuilian Liu[1], Xu Jia[1], Rens Ham[2], Chongting Ren[1], Luc Van Meervelt[1], Joost N. H. Reek[2], Tatjana N. Parac-Vogt[1]

[1]Dept. of Chemistry, KU Leuven, Belgium; [2]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands

The confinement effects within coordination cages present powerful tools in modern chemistry, particularly for the synthesis and manipulation of complex molecules. The extension of these phenomena to larger and more complex metallic clusters, such as polyoxometalates (POMs), has only recently been explored, yet it may hold large potential. POMs represent a unique class of anionic metal-oxygen clusters with special characteristics that have been extensively investigated for various applications. In these works, we employ host-guest stabilization within a coordination cage to enable a novel cavity-directed synthesis of labile POMs in aqueous solutions. Importantly, the encapsulation of these POMs enhances their stability in water, rendering them efficient catalysts for environmentally friendly and selective sulfoxidation reactions. Moreover, the developed host-guest approach facilitates POM-templated self-assembly of new robust coordination cages from a kinetically inert metal and conformationally mismatched ligands. These efforts expanded the supramolecular concept beyond traditional chemistry, demonstrating its significant potential to advance the field of metallic clusters and coordination cages, and to unlock new possibilities for sustainable catalysis and functional materials.

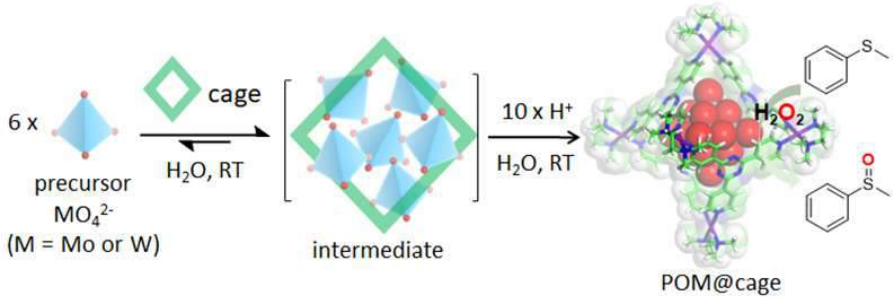

Fig. 1. Schematic representation of the cavity-directed synthesis of labile Lindqvist $[M_6O_{19}]^{2-}$ (M = Mo, W) POMs through encapsulation within a coordination cage and used as a supramolecular catalyst.

We thank Research Foundation Flanders (FWO), KU Leuven and the University of Amsterdam for financial and infrastructure support.

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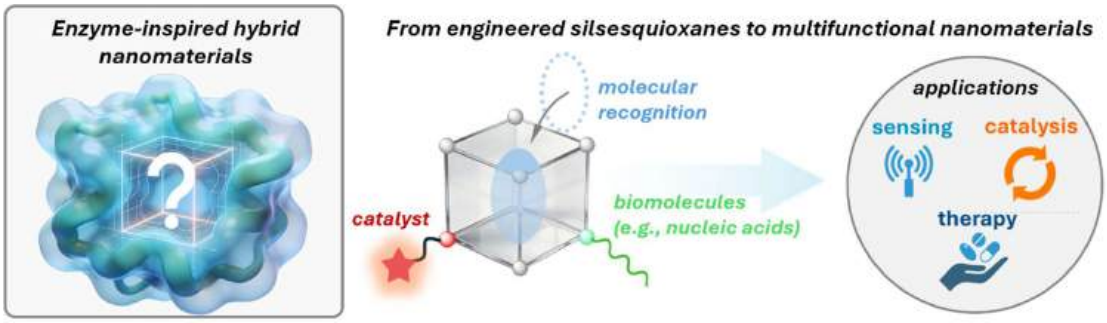
MDR - D1 - O06

Designing nature-inspired multifunctional nanomaterials through silsesquioxane chemistry

Pierre Picchetti[1], Rabia Zahid[1], María Sancho-Albero[2], Alessandro Porchetta[3]

[1]Karlsruhe Institute of Technology, Germany; [2]CISC-University of Zaragoza, Spain; [3]University of Rome Tor Vergata, Italy

Nanomaterials have established a remarkable success story and now play central roles in areas ranging from catalysis to drug delivery and vaccine design.[1,2,3] The next transformative step in the field will rely on multifunctional systems capable of performing coordinated tasks while approaching the structural and functional complexity of enzymes. Achieving this goal demands precision-chemistry strategies that deliver well-defined architectures with controlled functionality and intrinsic biocompatibility. In this context, cubic silsesquioxanes emerge as versatile molecular building blocks for enzyme-like nanomaterials, as their inorganic cores can be decorated with multiple, spatially defined functional groups. In combination with rational molecular design, these nanoscale cubes can display enzyme-mimetic behavior, offering a modular platform for next-generation nanomedicines that integrate sensing, catalysis, and therapeutic functions within a single scaffold. Herein, new synthetic routes to water-stable, multifunctional cubic silsesquioxanes are presented, alongside selected examples that illustrate their performance in catalytic, recognition-based, and stimulus-driven processes in biologically relevant environments. The capacity of these constructs to couple precise synthetic control with biomimetic functions, including controlled assembly/disassembly and anticancer activity, positions them as a promising class of advanced biomedical nanomaterials with potential impact on next-generation theranostics.



Acknowledgements: The authors gratefully acknowledge the financial support provided by the Fonds der Chemischen Industrie (FCI) and the Spanish Ministry of Science, Innovation and Universities from the Spanish Government.

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MDR - D1 - O07
Stimuli-responsive amino acid-based surfactants as nanovectors for biomedical applications

M. Luísa C. do Vale[1], Sandra G. Silva[1], Pedro C. Cardoso[1], Isabel S. Oliveira[2], Eduardo F. Marques[2],
[1]LAQV-REQUIMTE, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Portugal;
[2]CIQUP-IMS, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Portugal

Cationic surfactants possess unique amphiphilic properties which confer them the ability to modulate the solubility, stability, and bioavailability of therapeutic molecules, making them valuable as drug/gene delivery systems, in vaccine formulations, in cancer treatment, and as antimicrobial agents [1]. However, the cytotoxicity exhibited by most conventional cationic surfactants has hampered their widespread use, and continuous efforts have been endowed to overcome this problem. A major step forward has been the incorporation of naturally derived motifs, such as amino acids, peptides, and carbohydrates, into surfactant architectures, a strategy that has substantially enhanced their biocompatibility and overall safety [2-4].
The present study focuses on the design and synthesis of a variety of amino acid-based amphiphiles, engineered for biomedical applications. Emphasis is given to the incorporation of cleavable bonds as well as pH and redox-sensitive groups to impart stimuli-triggered behaviour to these surfactants. Their physicochemical characterization (self-aggregation, DNA complexation, pH/redox sensitivity) will also be presented.

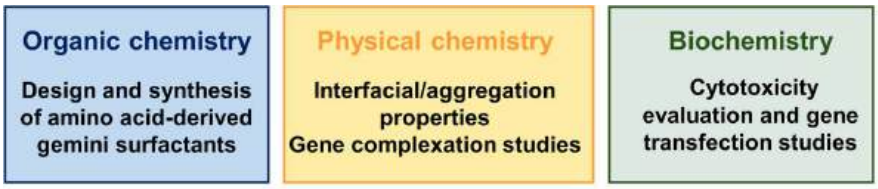

Figure. Workflow of the present study

Funding: This work received financial support from PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through project 20022.05543.PTDC – Smart4Vir.

Acknowledgements: Thanks are due to project UID/50006/2025 DOI 10.54499/UID/50006/2025 – Laboratório Associado para a Química Verde – Tecnologias e Processos Limpos. SGS acknowledges FCT for researcher employment contract CEEIND/01932/2017/CP1427/CT0003. P.C. thanks FCT for BI-research grant REQUIMTE 2023-54.

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MDR - D1 - O08

Enantioselective radical synthesis of β-lactams via Co(II)-based metalloradical catalysis enabled by ligand innovation

Many Hemati[1], Mariah Tedder[1], Duo-Sheng Wang[1], X. Peter Zhang[1]
[1]*Dept. of Chemistry, Boston College, USA*

β-Lactams represent a unique class of *N*-heterocyclic compounds with both fundamental importance and biological significance. Differing mechanistically from previous methods, we report herein a catalytic radical approach for stereoselective construction of chiral β-lactams via Co(II)-based metalloradical catalysis (MRC [1]). Supported by a newly-designed D_2-symmetric chiral amidoporphyrin (Scheme 1), the Co(II)-based metalloradical system can activate readily accessible α-diazoamides for asymmetric 1,4-C–H alkylation, enabling stereoselective synthesis of β-lactams in high yields with high enantioselectivities. The Co(II)-catalyzed radical alkylation is applicable for diverse α-diazoamides with varied steric and electronical properties, including those derived from drug molecules and natural products (Table 1). Through computational and experimental studies, we have elucidated the stepwise radical mechanism for Co(II)-catalyzed 1,4-C–H alkylation, involving the uncommon steps of 1,4-hydrogen atom abstraction (HAA) and 4-exo-tet radical substitution (RS). We have demonstrated that the resulting β-lactams can be further transformed into valuable cyclic and acyclic compounds in excellent yields with retention of the original stereochemistry. As a specific application, the Co(II)-catalyzed enantioselective 1,4-C–H alkylation has been utilized as a key step in achieving asymmetric synthesis of the drug ezetimibe.

Scheme 1. Ligand Effect on Co(II)-Based Catalytic System for Enantioselective 1,4-C–H Alkylation of α-Diazoamide

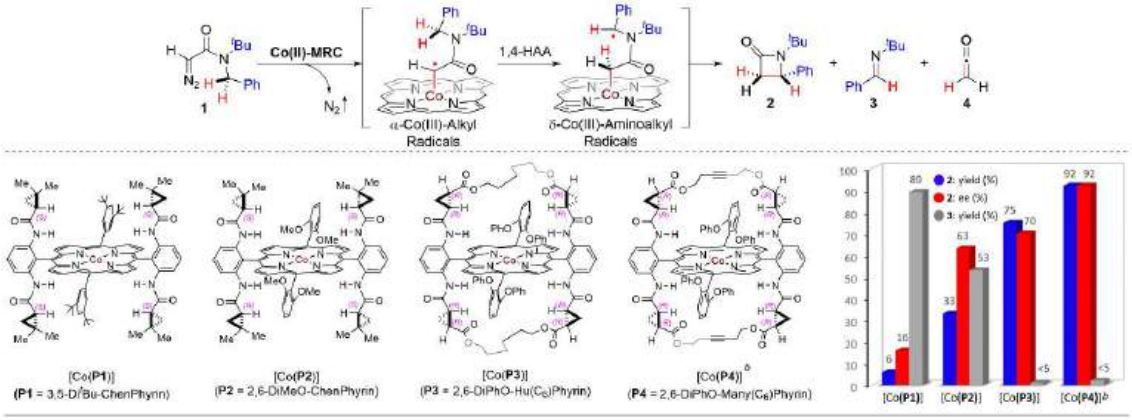
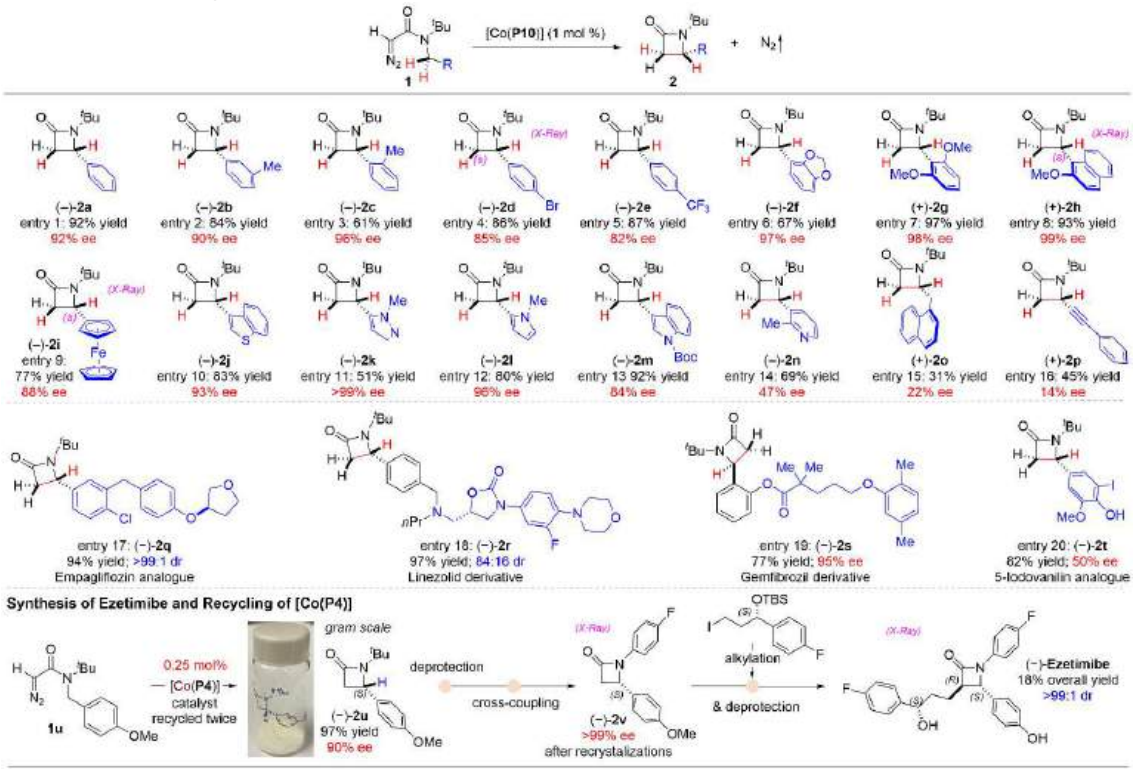


Table 1. Selected Scope for Enantioselective 1,4-C–H Alkylation of α–Diazoamides by Co(II)-Based System for Construction of β-Lactams



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MDR - D1 - O09
Moiré superlattices from bilayers of synthetic 2D polymers: On-surface synthesis and defects

Brecht Koek[1], Vipin Mishra[1], Veniero Lenzi[2], Karol Strutyński[2], Joaquín Almarza[3], Kunal S. Mali[1], Aurelio Mateo-Alonso[3], Manuel Melle Franco[2], Steven De Feyter[1]
[1]Division of Molecular Imaging and Photonics, Dept. of Chemistry, KU Leuven, Belgium; [2]CICECO—Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal; [3]POLYMAT, University of the Basque Country UPV/EHU, Donostia-San Sebastian, Spain

A 2D moiré superlattice forms when two or more atomically thin layers, such as graphene or transition metal dichalcogenides (TMDs), are stacked with a slight twist or lattice mismatch. This results in a moiré pattern with a periodicity much larger than the original lattice constants, giving rise to novel quantum properties. Moiré superlattices have revealed a range of exotic quantum phenomena, including flat electronic bands, the anomalous quantum Hall effect, unconventional superconductivity, and ferromagnetism. These discoveries underscore their transformative potential for future quantum technologies, as they provide a tunable platform bridging superconducting and insulating states.
Despite significant scientific progress, a major challenge remains: the lack of a general and efficient method for producing high-quality 2D moiré materials. In this contribution we explore the potential of synthetic 2D polymer bilayers, created via on-surface synthesis, as alternatives to graphene- or TMD-based moiré superlattices. Firstly, we look into how on-surface synthesis, combined with scanning tunneling microscopy (STM), enables the characterization of the structural and dynamic properties of synthetic 2D polymers. Finally, we discuss our recent findings on the formation of moiré superlattices in synthetic 2D polymers, especially the formation of defects within such moiré bilayers.

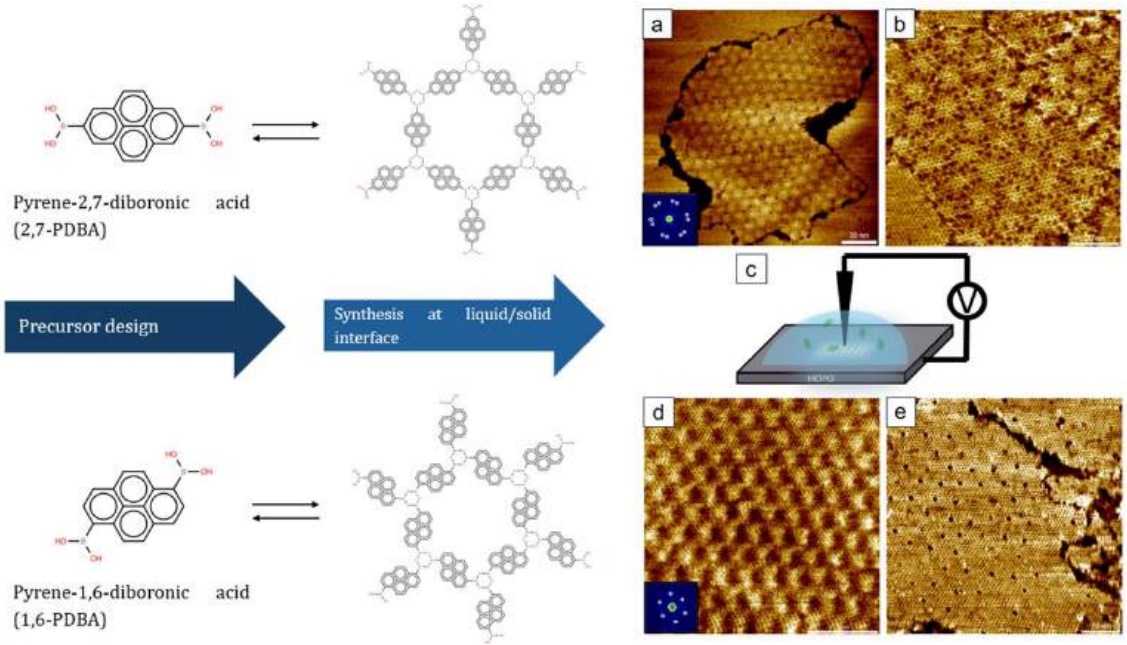

Fig. 1. a) STM image of 2,7-PDBA with a moiré domain surrounded by non-moiré domain b) STM image showing defect formation in 2,7-PDBA moiré domain c) Scheme illustrating in-situ STM measurement of COF formation d) STM image of 1,6-PDBA showing an extended moiré pattern e) STM image of 1,6-PDBA moiré domain revealing formation of periodic defects

MDR - D1 - O10

Tailored 2D covalent organic frameworks with ambipolar repeating units as cathode material for aluminum energy storage device

Cataldo Valentini[1*], Verónica Montes-García[1], Wojciech Kukułka[1], Saira Sarwar[1], Michał Bielejewski[2], Mateusz Wlazło[3], Rossella Greco[4], Viktorija Pankratova[4], Ignacio Pérez Juste[5], Dawid Pakulski[1], Paolo Samorì[6], Artur Ciesielski[1,5]

[1]Centre for Advanced Technologies, Adam Mickiewicz University, Poznań, Poland, [2]Institute of Molecular Physics Polish Academy of Sciences M., Poland; [3]Chemical and Biological Systems Simulation Lab Centre of New Technologies, Poland; [4]Nano and Molecular Systems Research Unit, University of Oulu, Finland; [5]Dept. of Physical Chemistry, Campus Universitario As Lagoas-Marcosende, Spain; [6]Université de Strasbourg and CNRS, ISIS, France

Covalent organic frameworks (COFs) represent a rapidly growing class of crystalline porous polymers whose properties can be precisely tailored through molecular design and controlled reactivity.[1] Constructed from organic building blocks linked by dynamic covalent bonds, COFs combine long-range structural order, permanent porosity, high-surface area and modular chemical composition. These features make them ideal platforms for studying fundamental structure-property relationships and for the rational creation of functional materials for energy storage applications.[2,3] However, the limited electrical conductivity of COFs makes essential the use of additives (such as carbon nanotubes) to increase the ions mass transport and electrical conductivity. To overcome this problem, the deliberate integration of electron-rich and electron-deficient units within COFs offers opportunities to engineer charge-transfer pathways, tune redox activity, and enhance electronic communication across the framework.[4,5] Here, we address this challenge through the molecular design of a two-dimensional donor-acceptor imine-linked COF constructed from electron-rich tetrakis(4-aminophenyl)-1,4-phenylenediamine (TPA) and electron-deficient naphthalenediimide dialdehyde (NDI-DA) units. The resulting framework exhibits high crystallinity, well-defined nanopore of 1.6 and 3.4 nm, and a large specific surface area (924 m^2/g). The planar geometry of the building blocks promotes an extended π-conjugated network and ordered stacking, while morphological studies reveal a robust nanotubular architecture proving the eclipsed stacking. Importantly, the rational donor-acceptor pairing induces intrinsic charge-transfer interactions within the framework, providing efficient electronic pathways without the need for external conductive additives, such as carbon nanotubes. When employed as a cathode in aluminum-ion energy storage systems, the COF TPA-NDI displays high specific capacity (270 mAh/g), and outstanding long-term cycling stability (over 5000 cycles). The ambipolar nature of the COF TPA-NDI allows reversible coordination of both cationic and anionic species, which was proved by in situ x-ray photoemission spectroscopy of the charged and discharged cathode.

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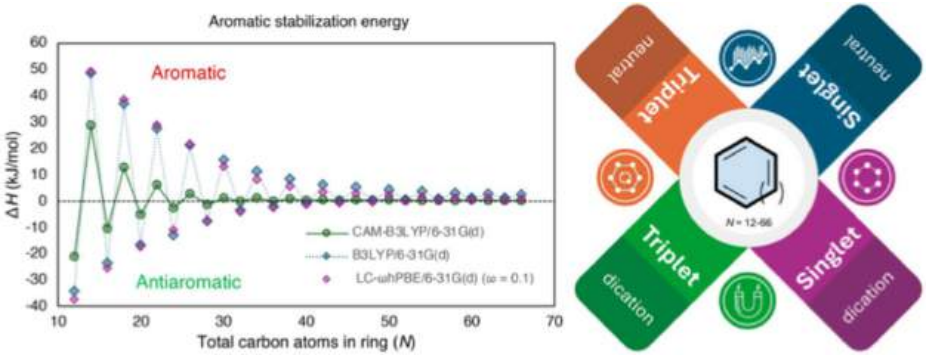
MDR - D1 - O11
Effect of size, charge, and spin state on Hückel and Baird aromaticity in [*N*]annulenes

Louis Van Nyvel,[1,2] Mercedes Alonso,[1] Miquel Solà[2]
[1]Dept. of General Chemistry (ALGC), Vrije Universiteit Brussel (VUB), Belgium; [2]Institut de Química Computacional i Catàlisi (IQCC), Dept. de Química, Universitat de Girona, Spain

Aromaticity is intricately linked to properties such as conductance and diradical character, underscoring its broad significance.[1,2] Understanding the principles that govern aromaticity across different electronic states is essential for rationalising its impact. The Hückel and Baird rules provide a conceptual framework for monocyclic π-conjugated systems in their singlet ground and lowest-lying triplet states, respectively, particularly in the context of [*N*]annulenes. According to Hückel's rule, a ground-state molecule is aromatic when it contains (4n+2) π-electrons, whereas Baird's rule predicts aromaticity in the lowest-lying triplet state for systems with (4n) π-electrons (n = 0, 1, 2, …).



A previous study explored how aromaticity evolves in singlet ground-state [*N*]annulenes as ring size increases from *N* = 12 to 66.[3] However, no systematic investigation has yet been conducted for the lowest-lying triplet state of [*N*]annulenes or their charged counterparts. In this work, we addressed this gap by performing DFT calculations across several aromaticity descriptors, with a particular focus on aromatic stabilisation energies (ASEs).[4] Our findings reveal that both neutral and charged [*N*]annulenes adhere to the Hückel and Baird rules. Nevertheless, for larger rings, these rules diminish in significance,[5] and the distinction between ASEs (and other indices of aromaticity) of [*N*]annulenes with (4n) and (4n+2) π-electrons becomes progressively less pronounced.

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MDR - D1 - O12
Reactivity models for tetrazine-based bioorthogonal reactions

Dennis Svatunek[1], Tori Demuth[1]
[1]TU Wien, Institute of Applied Synthetic Chemistry, Austria

Bioorthogonal chemistry describes reactions that combine exceptional reactivity with high selectivity under biologically compatible conditions. Among these transformations, tetrazine ligations stand out as some of the fastest bioorthogonal reactions known. Rational optimization of their reactivity remains challenging due to the interplay of electronic, steric, and strain effects that jointly determine reaction rates. In many cases, increasing reactivity comes at the expense of molecular stability.
In our research, we combine computational analysis with experimental kinetics to obtain a detailed mechanistic understanding of the factors controlling reactivity and stability in bioorthogonal tetrazine reactions. These insights are condensed into simplified, chemically intuitive reactivity models that enable rational design rather than empirical screening.
Representative systems used to develop such reactivity models are shown in Figure 1. In 2-pyridyl-1,2,4,5-tetrazines, reactivity is enhanced without compromising stability due to a repulsive lone-pair–lone-pair interaction in the reactant state. Cyclopropane-fused dibenzocyclooctynes display high reactivity toward tetrazines as a result of enforced reactive conformations, whereas the parent dibenzocyclooctynes remain essentially unreactive. In 4-hydroxy-substituted trans-cyclooctenes, reactivity is reduced by a transannular π→σ* interaction when the hydroxy group occupies an equatorial position, while an axial orientation leads to increased reactivity due to intramolecular Pauli repulsion.

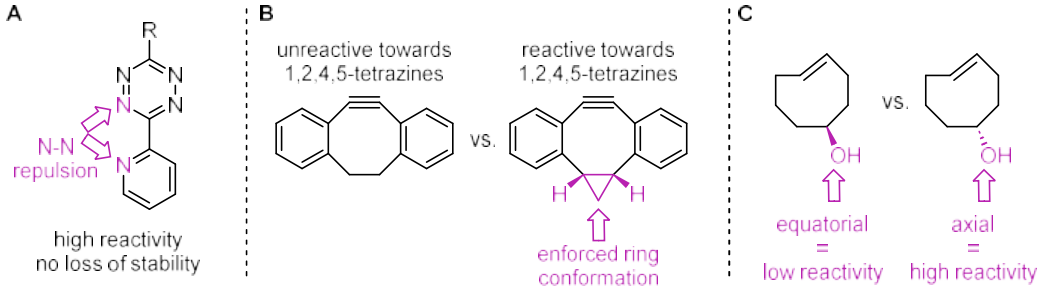

Fig. 1. Reactivity trends in tetrazine ligations arising from **A)** lone-pair repulsion,[1] **B)** enforced conformations,[2] and **C)** stereoelectronic effects in representative systems.

In this contribution, we discuss how mechanistic insight into tetrazine ligation reactions can be translated into simplified reactivity models that support rational reaction design and help identify strategies to improve bioorthogonal performance beyond empirical trial-and-error.

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MDR - D1 - O13
Molecular design beyond the frontier molecular orbital picture

Felix Plasser
Loughborough University, Loughborough, UK

Molecules able to absorb and emit light play a central role in modern science for the development of efficient light sources and solar cells as well as for scientific tools, such as fluorescent labels, sensors, and probes. Tremendous effort is invested in developing optimized molecules for these applications. To date only a small number of design rules exist, mostly based on the energies and shapes of the frontier molecular orbitals (FMO), meaning that extensive screening is often necessary. It is the purpose of this work to highlight two alternative strategies, going beyond the standard FMO picture, to explain photophysical behavior and ultimately design new molecules: (i) modulation of singlet-triplet gaps via the transition density, and (ii) tuning of excitation energies via excited-state aromaticity.

We have shown that the transition density provides an intuitive way for explaining, both, optical brightness and singlet-triplet gaps of π-conjugated chromophores.[1] Applied to the case of singlet fission, this framework was used to devise three now rules for maximizing S_1/T_1 gaps: (i) reducing the number of π-electrons, (ii) localizing the excited electrons within the π-system, and (iii) optimizing specific through-space interactions.[2,3] We highlight the applicability of this model bridging from simple hydrocarbon backbones to realistic dyes. As a second example, we will investigate the effects of excited state aromaticity and its spectroscopic signatures, such as particularly large Stokes shifts, on a set of macrocycles.[4] Finally, a new set of dyes with Stokes shifts of more than 2 eV will be presented, designed using the concept of excited state aromaticity gain.[5] Combined, we hope that these examples illustrate the power of going beyond the standard FMO picture opening new horizons for designing chromophores.

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[4]Eder, S.; Ding, B.; Thornton, D. B.; Sammut, D.; White, A. J. P.; Plasser, F.; Stephens, I. E. L.; Heeney, M.; Mezzavilla, S.; Glöcklhofer, F. *Angew. Chemie Int. Ed.* **2022**, *61*, e202212623.
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MDR - D1 - O14
SURFF: A new simple, universal and robust force field for large-scale molecular modeling in ORCA

Bernardo de Souza[1], Markus Bursch[1], Hagen Neugebauer[1], Christoph Plett[1], Christoph Riplinger[1]
[1]FACCTs GmbH, Germany

Here we introduce SURFF (Simple, Universal and Robust Force Field), a physics-based force field designed for fast and stable molecular modeling across a wide range of chemical systems. SURFF is built around a compact functional form with a small number of global parameters and does not require atom-specific parametrization. Its main design goals were robustness, transferability, and linear-scaling performance across the entire periodic table, which was achieved and will be demonstrated in this presentation.
The energy expression includes electrostatics, polarization, dispersion, and Pauli repulsion. Directional effects arising from lone pairs, π systems, and σ-holes are treated explicitly through angular modulation of both attractive and repulsive terms. This allows SURFF to describe hydrogen-bond directionality, anisotropic short-range repulsion, and geometrical distortions without introducing element- or environment-dependent parameters.
SURFF has been evaluated on large benchmark sets covering conformational energies, torsional profiles, and noncovalent interactions. On these targets, the accuracy is comparable to established force fields and, in many cases, approaches that of modern semiempirical methods like GFN2-xTB[1], while remaining significantly cheaper computationally. The physically motivated construction leads to stable behavior outside the benchmark domain, which is essential for structure exploration.
The method is implemented as a plugin to the ORCA[2] program package and scales linearly with system size. Due to its low computational and memory overhead, SURFF can be applied to systems ranging from small molecules to very large molecular assemblies, including systems with several hundred thousand atoms. Within ORCA, SURFF can be used for structure generation, conformational sampling, QM/MM and docking-type applications, and serves as an efficient pre-screening step prior to higher-level electronic structure calculations.

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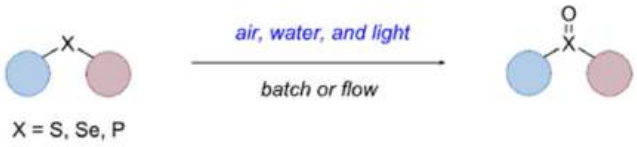
MDR - D1 - O15
Scalable and sustainable heteroatom oxidation in continuous flow

Koen Van Aken[1], Damiano Diprima[2], Stefano Bonciolini[2], Hannes Gemoets[3]
[1]Creaflow, Belgium; [2]University of Amsterdam, The Netherlands; [3]HT, The Netherlands

Although oxidation reactions are fundamental to the chemical industry, they are traditionally hampered by poor selectivity, severe safety hazards, and a heavy environmental footprint.
This work introduces a sustainable, catalyst-free oxidation methodology for heteroatoms (including S, P, and Se) that operates using air, water, and light[1]. Furthermore, we propose a novel reaction pathway demonstrating that the incorporated oxygen originates directly from water, offering unique mechanistic insights. To validate its industrial viability, the batch protocol was seamlessly transitioned into continuous flow using the HANU reactor.



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MDR - D1 - O17

Turning oxetanes into predictable building blocks through reactivity and physchem mapping

Eduard Litskan[1,2], Dmytro Granat[1,2], Bohdan Vashchenko[2,3], Dmytro Leha[2,3], Dmytro Volochnyuk[1,2,3,4], Serhiy V. Ryabukhin[1,2,3,4]

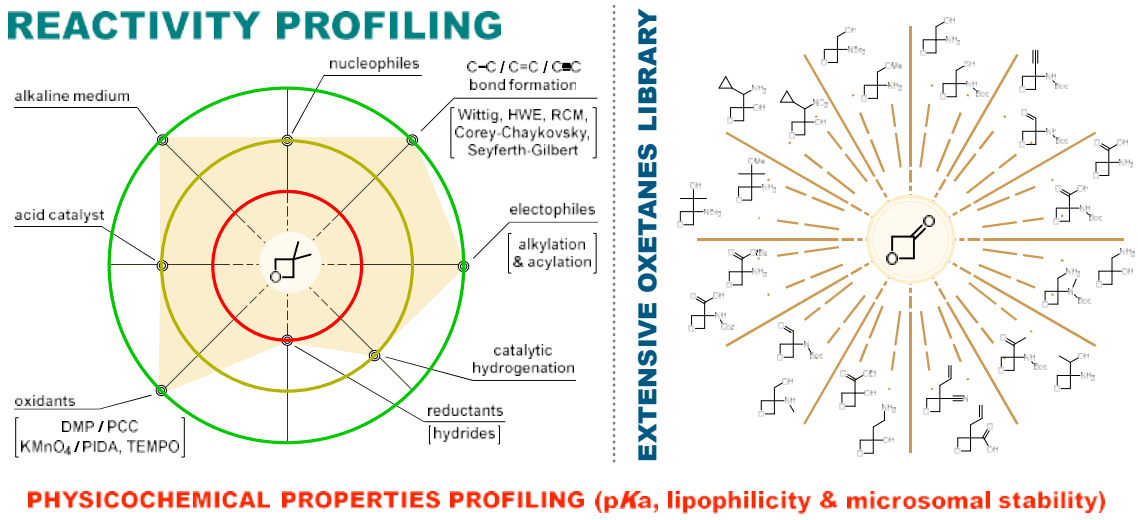
[1]Enamine Ltd, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Scientific Research Institute, Ukraine; [4]Institute of Organic Chemistry, NAS of Ukraine

Oxetanes have become one of the most attractive sp3-rich motifs in medicinal chemistry because they can serve as a compact bioisosteric replacement for carbonyl and gem-dimethyl fragments while improving solubility, reducing lipophilicity, and reshaping metabolic stability. Yet, despite their high value, oxetanes still carry a reputation as “fragile fragments,” as the strained four-membered ring is prone to ring opening, particularly under acidic or strongly nucleophilic conditions, complicating synthesis, purification, and even storage. This instability ultimately limits the availability of simple, affordable 3,3-disubstituted oxetane building blocks.

Here, we report a comprehensive program that tackles this bottleneck from two angles: (1) scalable access to diverse 3,3-disubstituted oxetanes and (2) systematic understanding of how the oxetane core and its substitution control reactivity, stability, and physicochemical parameters. The work was designed as a reaction-profile study, mapping oxetane tolerance across typical transformations used in medicinal chemistry (oxidation, reduction, alkylation, acylation, nucleophilic substitution, C-C bond formation, hydrolysis, and deprotection), including challenging acid-mediated cases.

In parallel, physicochemical profiling demonstrates that oxetanes can act as a property engineering module. In particular, oxetane incorporation decreases amine basicity relative to cycloalkyl and gem-dimethyl analogues, while fluorination enables fine-tuning of lipophilicity and acidity.

In the report, we will discuss design rules for oxetane building blocks, reaction condition guidelines, and structure/property trends enabling predictable MedChem optimization.



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MDR - D1 - O18
Simulating proteins with disulfide bonds under reducing conditions

Dilsah Nur Elmaci[1], Gene Hopping[2], Markus Muttenthaler[2,3], Matthias Stein[1]
[1]Max Planck Institute for Complex Technical Systems, Germany; [2]University of Queensland, Australia; [3]University of Vienna, Austria

Six conserved cysteine residues forming three intramolecular disulfide bonds stabilize the human TFF1 protein. These give the protein its characteristic trefoil factor structure. TFF1 shows a remarkable stability against increasing concentrations of the reducing agent tris(2-carboxyethyl)phosphine (TCEP). Full reduction of TFF1 was only achieved at large excess of TCEP (150-fold), and no partially reduced intermediates were observed, supporting a compact TFF1 domain. This TFF1 domain stability was investigated by extensive all-atom molecular dynamics simulations for a total of 24 μs of all possible combinatorial states of disulfide bond reduction. Despite minor structural and conformational changes observed upon reduction, the domain substantially retained its overall compactness and solvent exposure when only one or two disulfide bonds were removed. The reductions of covalent disulfide bonds were treated using quantum chemical calculations to identify the order of reduction events. Loss of disulphide bonds upon reduction was compensated by persistent non-covalent interactions. This is a first insight into the remarkable stability of the human TFF domain under reducing conditions, supporting its functional resilience upon expression and secretion throughout the human body.[1]
As a reference, the drug molecule Linaclotide, which is used to treat irritable bowel syndrome and chronic idiopathic constipation is used. This small peptide also contains three intramolecular disulphide bonds. However, these are more easily reduced compared to TFF1. This explains the shorter lifetime of Linaclotide.

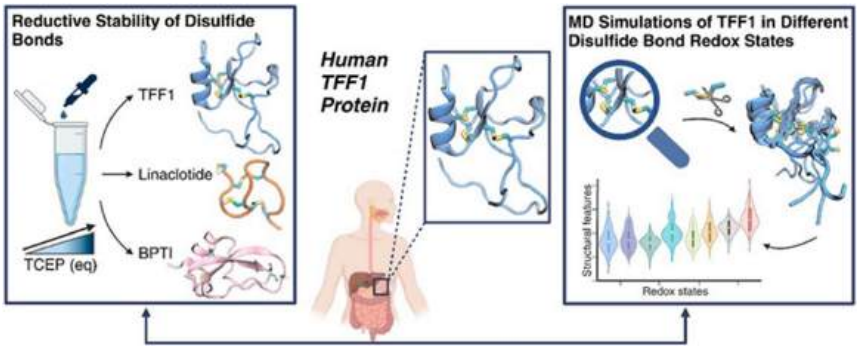

Fig. 1. Combined experimental and computational study of the stability of human TFF1 under reducing conditions.

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MDR - D1 - O19

Asymmetric synthesis of stereogenic-at-sulfur compounds via biocatalytic oxidation with unspecific peroxygenases

Jiacheng Li[1], Benjamin Melling[1], Katy A.S. Cornish[1,2], Nicholas Mulholland[3], Jared Cartwright[2], William P. Unsworth[1]*, Gideon Grogan[1]*

University of York, Depts. of Chemistry[1], and Biology[2] UK; [3]Syngenta, Jealott's Hill International Research Centre, UK

Biocatalysis has emerged as one of the most powerful catalytic toolboxes in organic synthesis.1 One Illustration of this is that complex molecules can be functionalized by oxygenase enzymes with high regio- and enantioselectivity.2 P450s, some of the most well-known oxygenases, are capable of oxidizing a range of compounds selectively. However, their use in preparative scale oxygenation is limited due to their dependence on NADPH and the auxiliary proteins needed for electron transfer. Unspecific Peroxygenases (UPOs), which were first discovered in 2004,3 have been identified as an effective alternative to P450s.as they, only rely on the addition of H2O2 to form the catalytic iron oxoferryl species 'Compound I' in the active site, giving them huge potential for applications to preparative scale reactions. To further explore the ability of the UPOs in organic synthesis, we describe the biocatalytic oxygenation of sulfilimines (1) and sulfenimines (3) to afford enriched sulfoximes (2) and sulfinimines (4) respectively, on preparative scale. In the sulfilimine series, sulfoximines are generated in up to 98% ee via kinetic resolution (Figure 1a). In the sulfenimine series, the selective synthesis of both (R)- and (S)-sulfinmine products can be delivered (both up to 99% ee), with different UPOs giving products with opposite enantioselectivity (Figure 1b). To our knowledge, both approaches had no known biocatalytic precedent. This methodology adds another highly efficient application of UPOs to a growing list of reactions that have significant potential for scale-up in an industrial context.4

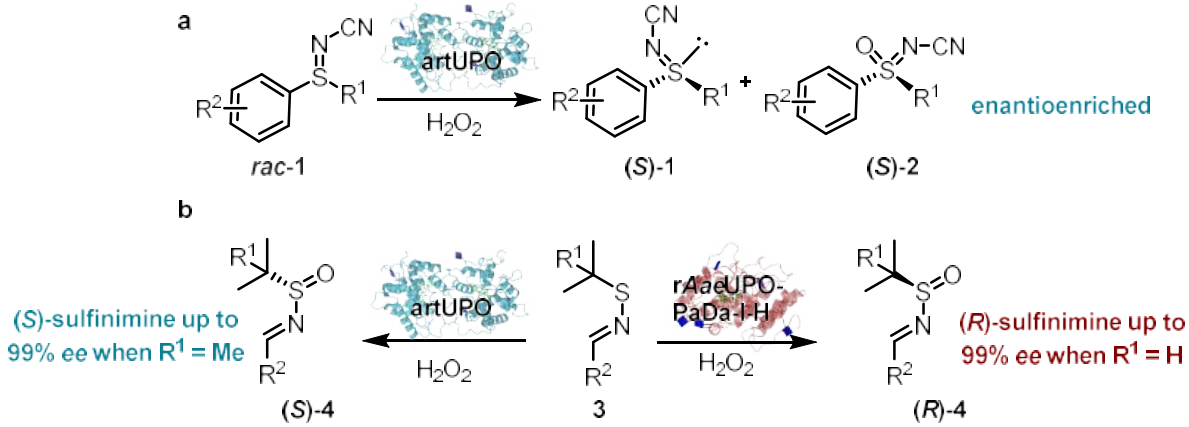

Fig. 1. Enantioselective sulfoximine and sulfinimine synthesis via UPO-catalysed oxygenation.

Keywords: Biocatalysis, Asymmetric synthesis, Sulfur, Unspecific Peroxygenase

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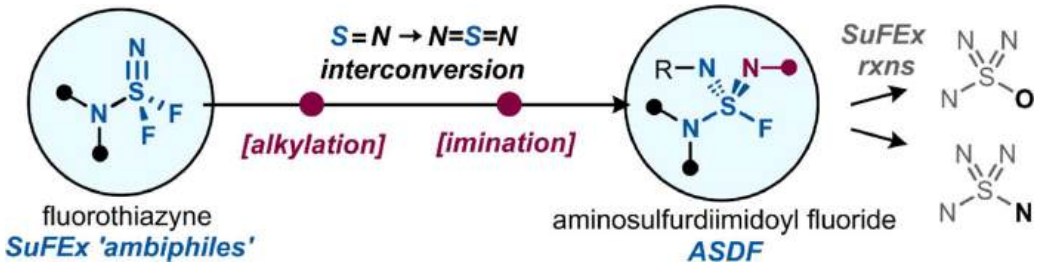
MDR - D1 - O21
Fluorothiazynes as SuFEx ambiphiles: Interconversion to aminosulfurdiimidoyl fluorides

Kexin Su[1], Luc Van Meervelt[1], Steven H.L. Verhelst[1], Wim M. De Borggraeve[1,*], Joachim Demaerel[1,*]
[1]KU Leuven, Belgium

Sulfur(VI) functional groups are ubiquitous in medicinal chemistry, valued for their stability and ability to modulate molecular properties. Over 130 S^{VI}-based drugs have been approved by the FDA, with sulfonamides, sulfones, and sulfates dominating existing drug scaffolds. Despite being a prevalent class of chemotypes in therapeutics, the sulfur(VI) core remains almost invariably the same: the sulfonyl (–SO_2–) group forms the centerpiece and acts as a two-directional linker between two other fragments. More recent work provides a strong case for the usefulness of three-directional linkers such as sulfurimidoyl- or thiazyl-based structures. However, a modular way to construct four-directional sulfurdiimidoyl structures is still wanting.



Here, we show a viable route from amino difluorothiazynes to aminosulfurdiimidoyl fluorides (ASDFs), via sequential alkylation and imination. Leveraging the ambiphilic character of fluorothiazynes—acting as both N-nucleophile and S-electrophile—we generate thiazynium intermediates that, upon trapping with primary amides or sulfonamides, afford ASDFs in good yields. Additionally, the potential of ASDFs as SuFEx electrophiles is demonstrated by reaction with various nucleophiles. Notably, a sulfurdiimidamide derivative was generated which is likely the first unsymmetrically substituted tetraimidosulfur species. This work expands the toolkit of azasulfur(VI) fluorides, introducing the first general route to ASDFs as stable, functionally diverse platforms for further chemical diversification.

[1]K. Su, L. Van Meervelt, S. H. L. Verhelst, W. M. De Borggraeve, J. Demaerel, *Angew. Chem. Int. Ed.*, **2025**, e23033. https://doi.org/10.1002/anie.202523033

MDR - D1 - O22
Synthetic strategies for building and editing nucleoside analogues

Michael W. Meanwell
University of Alberta, Canada

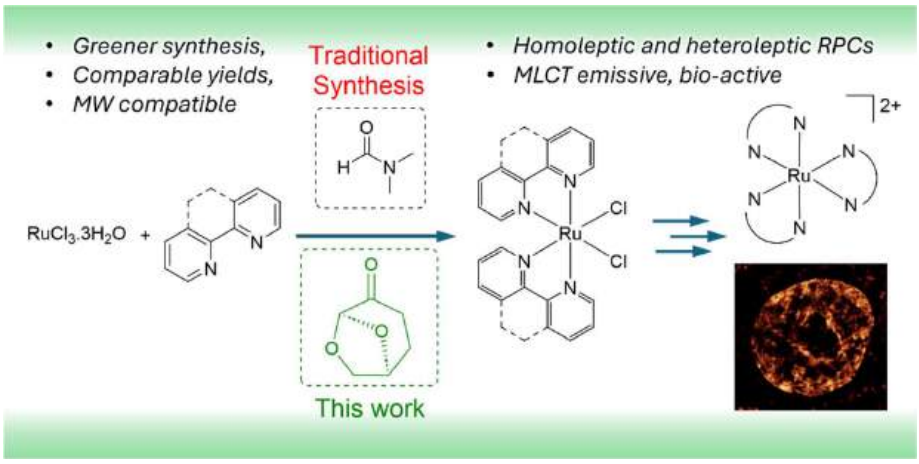
Nucleoside analogues (NAs) continue to be a central focus of drug discovery efforts worldwide due to their well-established impact on human health. With more than six decades of intensive research in this area, and a renewed surge of activity in recent years, the accessible chemical space of NAs has become increasingly saturated, making the identification of novel NA-based therapeutics progressively more challenging. Classical approaches to nucleoside analogue (NA) synthesis often suffer from poor modularity and lengthy synthetic routes, thus limiting rapid library generation. As a result, improved chemical methods are needed to streamline the synthesis of “hard-to-make” NAs, thereby increasing the efficiency with which NA chemical space can be explored to enable the discovery of new NA chemotypes. This seminar will highlight our laboratory’s efforts to develop de novo synthesis and molecular editing platforms that reduce step counts by up to 80% while providing access to previously untapped, yet pharmacologically relevant, NA chemical space.

This research was funded by the Alberta Ministry of Technology and Innovation through SPP-ARC (Striving for Pandemic Preparedness — The Alberta Research Consortium) and by GlycoNet, which is supported by the federal government’s Strategic Science Fund.

MDR - D1 - F01
Green(er) synthesis of MLCT-emissive ruthenium(II) polypyridyl complexes

Martin R. Gill[1]
[1]*Swansea University, UK*

Due to their flexible coordination chemistry, tuneable redox behaviour, stability in aqueous media, ability to emit from long-lived MLCT (metal to ligand charge-transfer) states, and capacity to bind biological targets with high selectivity, ruthenium(II) polypyridyl complexes (RPCs) find widespread use as luminescent probes and emerging bio-therapeutic agents.[1-3] Their versatility underpins a diverse range of applications including photocatalysis, light-harvesting, molecular and cellular imaging, and anticancer therapy.
Conventional synthetic routes to RPCs rely heavily on N,N′-dimethylformamide (DMF), a dipolar aprotic solvent designated a Substance of Very High Concern (SVHC) under EU REACH legislation. Its use presents a major obstacle to sustainable, large-scale production in compliance with the twelve principles of green chemistry. Here, we report a microwave-assisted, two-step synthesis employing Cyrene™ (dihydrolevoglucosenone), a biorenewable cellulose-derived solvent, as a direct and effective substitute for DMF in both the preparation of the key cis-$Ru(N^N)_2Cl_2$ precursor complexes and the subsequent formation of homoleptic $[Ru(N^N)_3]^{2+}$ type complexes (including the benchmark luminophore $[Ru(bpy)_3]^{2+}$) and heteroleptic $[Ru(N^N)_2(N'N')]^{2+}$ type complexes. Two novel methylated intercalators, $[Ru(bpy)_2(10,11\text{-dmdppz})]^{2+}$ and $[Ru(5,5'\text{-dmbpy})_2(10,11\text{-dmdppz})]^{2+}$, were synthesised using this route. Both exhibited exceptionally high DNA-binding affinities and pronounced MLCT luminescence enhancement upon intercalation, moderate cytotoxicity towards cancer cell lines and compatibility with advanced imaging techniques such as STED microscopy.[4]
Placed in the context of the sustainable manufacture of metallodrugs and imaging agents, challenges of extending this approach to hydrophobic ligand systems, solvent lifecycle, and promoting broader adoption of green synthetic practices in coordination and organometallic chemistry will be discussed.



We thank the Royal Society of Chemistry for funding.

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MDR - D1 - F02

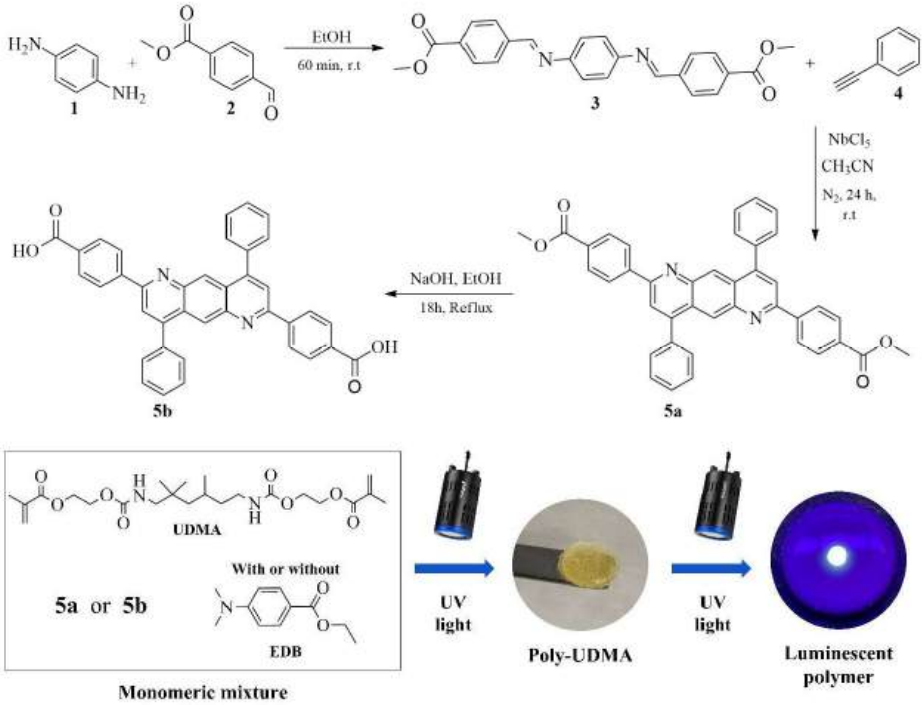
Anthrazoline derivatives as photoinitiators for photopolymerization reactions: studies about the synthesis and application

Emily B. Barros,[1] Ilana S. Rosário,[1] Caroline Gaglieri,[1] Luiz C. Silva-Filho[1]

[1]School of Sciences, Department of Chemistry, São Paulo State University (UNESP), Brazil

Anthrazolines are a class of aromatic aza-heterocycles that have gained attention due to their extended π-conjugated system, high thermal stability, and electronic properties that favor photoactive applications.[1] Among these applications, their potential use as photoinitiators is noteworthy, since photopolymerization has emerged as a fast, efficient, and energy-saving technique for polymer formation.[1] In this context, the aim of this work was to develop a new synthetic route using $NbCl_5$ to obtain new anthrazoline derivatives and evaluate their performance as photoinitiators in the photopolymerization of urethane dimethacrylate (UDMA).

In this work, we describe the new procedure to synthetize two anthrazoline derivatives in 3 steps. Firstly, the Schiff base ligand was prepared by condensing Methyl 4-formylbenzoate with 1,4-phenylenediamine in EtOH at room temperature (75%). This was followed by an aza-Diels–Alder reaction between the Schiff base and phenylacetylene promoted by $NbCl_5$ under mild conditions (39%, rt, 24 h). In the final step, the ester substituents were hydrolyzed, obtaining the diacid anthrazoline (88%). The structures were confirmed by MS, FTIR, and NMR. Both anthrazoline derivatives exhibited three absorption bands in the UV region (264, 321 and 351 nm), blue fluorescence, and high thermal stability, remaining stable above 360 °C. (Scheme 1)



Scheme 1: Synthesis and application of Anthrazoline derivatives as photoinitiators.

A comparative evaluation of the anthrazoline derivatives as photoinitiators operating via Type I or II mechanisms for the photopolymerization of UDMA was tested, under UV light irradiation (370 nm), using EDB as co-initiator in type II systems. The results indicate both derivatives as interesting PI type II candidates, achieving 45 to 55% of polymer conversion with low concentration (0.7 % wt), within 300 s, resulting in rigid luminescent polymers with blue light emission. (Table 1)

Table 1: UDMA-to-polymer degree of conversion (DC %) using Anthrazoline derivatives **5a** and **5b** as PI.

Entry	% PI (% wt)	DC (%)			
		PI **5a**	PI **5a** + EDB*	PI **5b**	PI **5b** + EDB*
1	1.0	29.2	39.4	34.4	45.5
2	0.7	35.7	45.6	36.3	55.3
3	0.5	37.6	44.7	36.9	49.7
4	0.3	38.0	43.7	36.6	46.8
5	0.1	38.8	44.3	31.8	50.2

*EDB % = 0.5 % wt

The authors would like to thank FAPESP [Grant numbers 2024/02435-1, 2024/00779-2, 2024/02935-1, 2025/27044-5), CNPq [Grant number 303750/2024-3] and CAPES.

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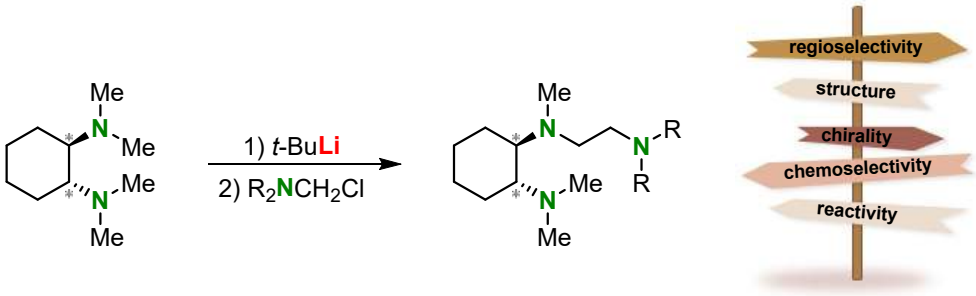
MDR - D1 - F03

Design of chiral ligands based on the reaction of α-functionalized lithium alkyls with iminium salts

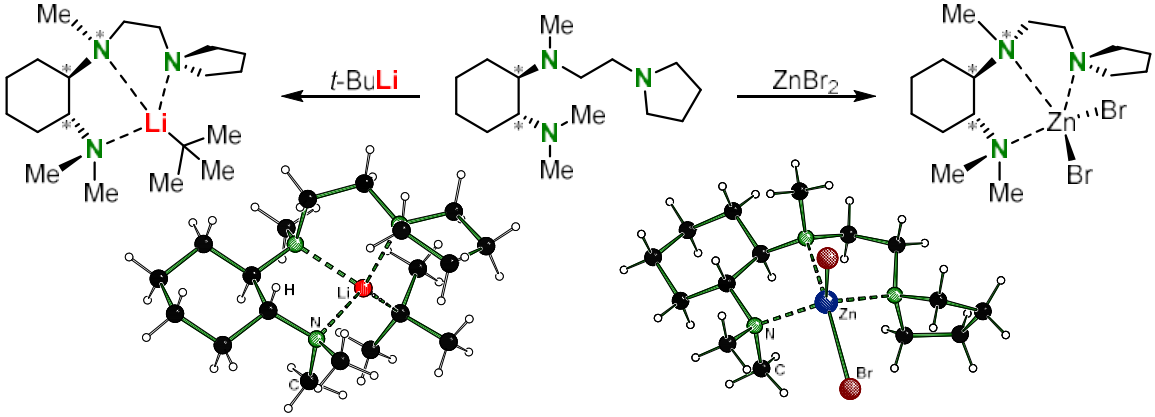
Tristan Mairath[1], Carsten Strohmann[1]
[1]Faculty of Chemistry and Chemical Biology, TU Dortmund University, Germany

The reactions of *α*-lithiated (*R*,*R*)-*N*,*N*,*N*',*N*'-tetramethylcyclohexane-1,2-diamine with methylene iminium salts ($R_2NCH_2^+Cl^-$) provide access to a series of chiral, novel, tridentate ligand systems.[1]



Scheme 1: Deprotonation of (*R*,*R*)-TMCDA with *tert*-butyllithium and addition to methylene iminium salts. (R = alkyl)

When these ligands coordinate a metal, a stereogenic nitrogen center is formed due to four different substituents at one nitrogen of (*R*,*R*)-TMCDA. The absolute configuration of the corresponding complex can be manipulated with the right choice of metal.[2] Defined configurations at the stereogenic nitrogen center are necessary to avoid the formation of mixtures or diastereomers for further transformations or catalytic applications.



Scheme 2: Crystal structures of (*R*,*R*)-trimethyl(pyrrolidinoethyl)cyclohexane-1,2-diamine coordinating to *tert*-butyllithium (left) and zinc bromide (right).

We are interested in the coordination of simple transition metal salts (for example $ZnBr_2$; possible catalyst for lactide polymerization[3]) and the main group element lithium in simple lithium alkyls. To overcome suppressed reactivities of higher alkyllithium aggregations, the focus is on monomeric, chiral alkyllithium aggregates with the tridentate ligands.[4,5] Stereogenic information can be transferred from chiral ligands with defined nitrogen configurations to the substrate.[6]

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MDR - D1 - F04
Molecular design of peptidic ligands for cortactin-SH3

Miriam Gulman*[1,2], Inbal Sher[1], Jordan Chill[1], Dan T. Major[1,2]
[1]Dept. of Chemistry, Bar-Ilan University, Israel; [2]Institute for Nanotechnology Advanced Materials, Bar Ilan University, Israel

Cortactin is a cytoplasmic protein that regulates actin polymerization and cytoskeletal rearrangement. Upon activation, it stabilizes nucleation sites for actin branching and is essential for lamellipodia, invadopodia, migration, and endocytosis. The cortactin SH3 domain (CortSH3) recognizes proline-rich peptides containing the “PXXP” motif, such as those from Proline-rich tyrosine kinase 2 (Pyk2) and hematopoietic cytoskeleton regulator WIP[1]. Our objective is to identify peptides with improved affinity for CortSH3 and better stability. These competitors block cortactin activation and thereby suppress lamellipodia and invadopodia assembly in cancer cells—key structures that drive motility, matrix degradation, and invasion. By inhibiting CortSH3 interactions, we aim to reduce metastatic potential while also probing how peptide sequence influences binding affinity.

This research combines experimental and computational approaches. To measure binding affinities of peptides to CortSH3 and derive distance restraints we use surface plasmon resonance and Nuclear Magnetic Resonance spectroscopy. The distance restraints are incorporated into docking with HADDOCK[2] (High Ambiguity Driven DOCKing) to determine CortSH3–peptide structures and predict peptide orientation in the SH3 binding groove. In addition, we use deep-learning structure prediction models (AlphaFold[3], Chai-1[4], and Boltz-2[5]) to determine protein–peptide structures and guide structural analysis. To optimize this process, we developed a restraints scoring function that determines how many distance restraints are needed to accurately dock peptides to CorthSH3, thereby making structure determination more efficient.

Complementing experiments, in silico screening of 4,608 peptides identified several promising CortSH3 ligands. One peptide bound ~50-fold stronger than the original 12-residue Pyk2 segment, and key interacting residues were mapped. Several variants were synthesized and tested, revealing sequence-affinity relationships. Overall, this work identifies a potent CortSH3-binding peptide and provides design principles for inhibitors that block cortactin-driven cancer cell invasion.

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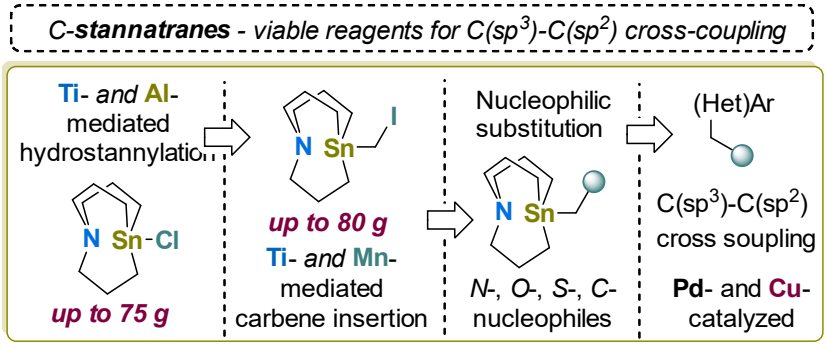
MDR - D1 - F05

Synthesis and application of alkylstannatranes: Versatile precursors for C(sp^3)-C(sp^2) cross-coupling

Oleksandr Liashuk[1,2], Oleksandr Zaporozhets[2,3], Pavlo Nosyk[2,3], Dmytro Sibgatulin[3], Oleksandr Grygorenko[1,2,3]

[1]Enamine SRI, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Ltd., Ukraine

Organostannane transformations are among the most versatile Pd-catalyzed cross-couplings, valued for their mild conditions and broad functional-group tolerance. Yet, ongoing safety concerns and the often limited accessibility of organotin reagents continue to constrain wider adoption. Organostannatranes (pentacoordinate tin species) offer a compelling compromise between stability, safety, and reactivity, but their broader use has been limited by the lack of dependable bulk-scale synthetic routes. Here we present a systematic study, from the preparation of the key precursor stannatranyl chloride to the identification of optimized cross-coupling conditions. Overall, our results position stannatrane derivatives as practical, readily accessible, and efficient reagents, expanding the plug-and-play toolkit of contemporary synthetic chemistry.



This work was supported by Enamine Ltd. O. Grygorenko and O. Liashuk received additional funding from Ministry of Education and science of Ukraine, grant No. 25BF037-01 (0125U002249).

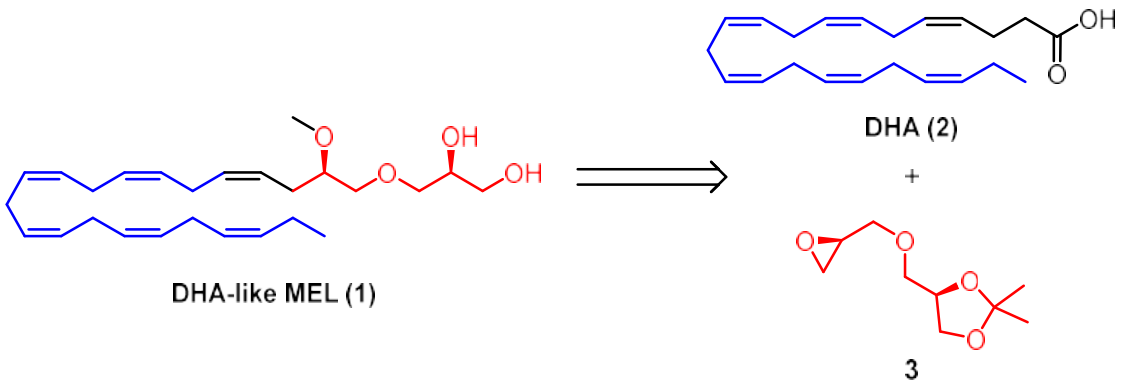
MDR - D1 - F06

Synthesis of n-3 polyunsaturated docosahexaenoic acid-like methoxylated ether lipid

Mina Bathen[1], Svanur Sigurjónsson[2], Karl E. Malterud[1], Daniel H. Hasselstrøm[1], Osman Gani[1], Anders Vik[1], Haraldur G. Guðmundsson[2], Guðmundur G. Haraldsson[2] and Trond V. Hansen[1]

[1]Univeristy of Oslo, Norway; [2]University of Iceland, Iceland

Docosahexaenoic acid (DHA)-like methoxylated ether lipid (MEL, **1**) is an unusual polyunsaturated ether lipid that contains six isolated *cis*-double bonds. It was first identified in 1971 in Greenland shark liver oil,[1] and has since been detected in both neutral lipids and phospholipids from human red blood cells.[2] The first total synthesis of this compound was reported in 2022 by Sigurjónsson *et al*.[3] Herein, a novel synthetic approach to DHA-like MEL **1** is reported. By utilizing a modular semi-synthetic approach, from natural DHA (**2**) and compound **3**, all six methylene skipped *cis*-configured double bonds were incorporated into the final product with high stereocontrol, affording an overall yield of 5.3% across 10-steps (longest linear sequence). In addition to the synthetic efforts, the biological relevance of DHA-like MEL **1** was further validated via molecular docking and molecular dynamics simulations with soybean 15-lipoxygenase-1. The simulations predict a moderate binding affinity (Glide score = -9.0 kcal/mol, MM/GBSA ΔG_{bind} = -60 kcal/mol), comparable to that of arachidonic acid. Finally, a biological assay with soybean 15-lipoxygenase-1 demonstrated that DHA-like MEL **1** is a substrate for the enzyme.



Scheme 1. **A retrosynthetic overview for the synthesis of DHA-like MEL 3.**

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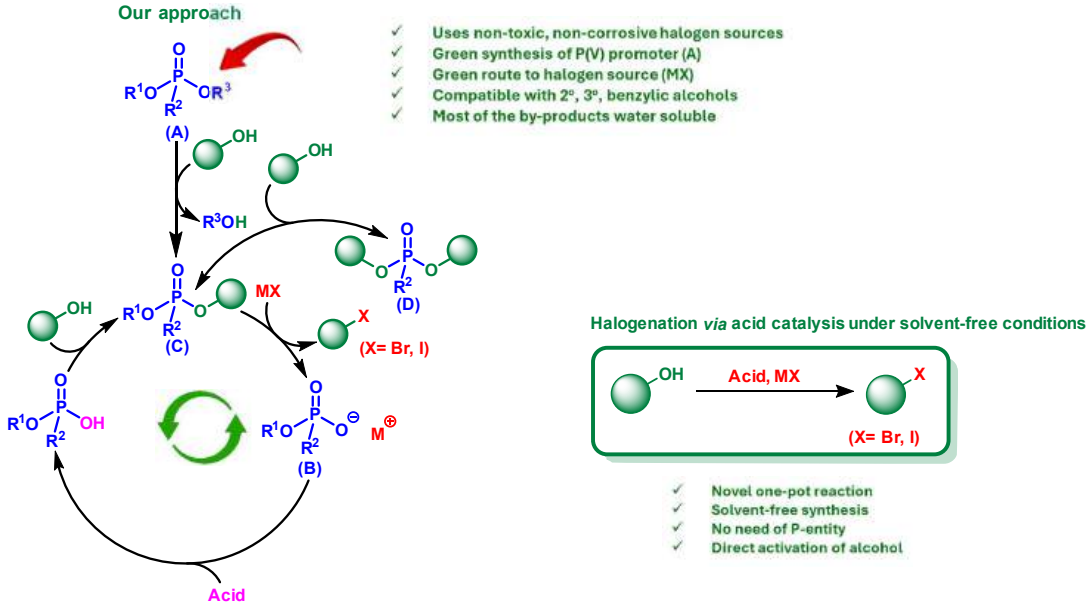
MDR - D2 - O01

Waste reduction and utilisation in alkyl halide synthesis: Development of "low waste" catalytic synthetic methodology

Ashwini Mishra[1], David Ryan[2], Aidan Cregan[2], Peter Byrne[1]*
[1]*School of Chemistry*, *University College Dublin, Ireland*; [2]*University College Cork, Ireland*

Alkyl halides are essential intermediates in organic, medicinal, and materials chemistry, yet their preparation often relies on hazardous reagents such as thionyl chloride and PBr_3, generating toxic and acidic waste. Similarly, the Appel reaction[1] suffers from poor atom economy due to stoichiometric phosphine oxide by-products. Although catalytic Appel-type halogenations have improved efficiency[2], the synthesis of required phosphorus reagents still produces significant halogenated waste. To address these challenges, we developed a greener halogenation protocol based on a bench-stable phosphorus promoter (**A**), prepared through a non-PCl_3-dependent synthetic route.[3]



We report a one-pot halogenation method that enables *in situ* regeneration of promoter (**A**) from its phosphorus by-product (**B**). Beginning with (**A**), sequential addition of acid, alcohol, and metal halide (MX, X = Br, I) allows conversion of two equivalents of alcohol per equivalent of promoter without isolating (**B**). This operationally simple protocol is effective for primary, secondary, and tertiary alcohols and represents a key step toward catalytic turnover of (**A**) in halide synthesis.

The methodology features several advantages: reduced waste generation, use of non-toxic halide sources, water-soluble by-products that simplify purification, and a modular one-pot setup. In addition, control experiments uncovered an unexpected acid-mediated halogenation pathway that proceeds without the phosphorus promoter. A subset of alcohols undergo efficient bromination and iodination under solvent-free conditions using only acid and metal halide, providing a complementary, minimal-waste strategy for specific substrates.

This work advances sustainable halogenation chemistry by coupling reagent recyclability with operational simplicity, offering a practical and environmentally accountable alternative to traditional alkyl halide syntheses.

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Taighde Éireann
Research Ireland

MDR - D2 - O02

Anchimeric assistance of acyl neighboring groups as stereodirecting strategy in synthesis: What can we learn from glycoscience?

Frank F.J. de Kleijne[1], Thomas J. Boltje[1]
[1]Institute for molecules and materials Radboud University, The Netherlands

Neighboring group participation (NGP) is a well-known concept in organic synthesis to modulate the reactivity of a molecule.[1] A famous example of a molecule that experiences high reactivity due to NGP is mustard gas. Another example of NGP is acyl participation (Figure 1, panel A). This type of NGP is useful for stereoselective synthesis. Typically, acyl NGP implies having a 1,2-relationship from participating to electrophilic side leading to transient five membered ring intermediates. In this work we ask ourselves the question: would participation from more remote positions such as in a 1,3-relationship be feasible to afford six membered ring intermediates (Figure 1, panel B)?

To answer this questions we turn our attention to glycoscience where C-2 acyl participation is commonly employed to prepare 1,2-*trans* glycosidic linkages (Figure 1, panel C).[2] For decades participation of acyl groups at C-3, C-4, and C-6 has been proposed but its existence remained heavily debated (Figure 1 panel D).[3] Only recently has direct experimental evidence become available for this phenomenon.[4,5,6] Herein we present our findings and report factors that enable 'remote' acyl NGP in order to predict if 'remote' acyl NGP would be feasible beyond the realm of glycoscience.

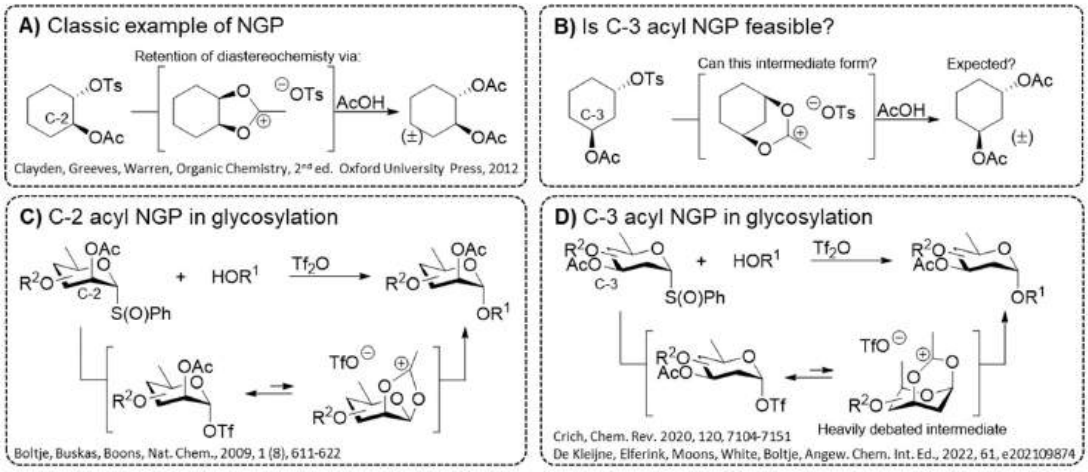

Fig. 1. A) Classic example of C-2 acyl NGP, **B)** Illustration of C-3 acyl NGP, **C)** Example of C-2 acyl NGP in glycosylation, **D)** Example of C-3 acyl NGP in glycosylation.

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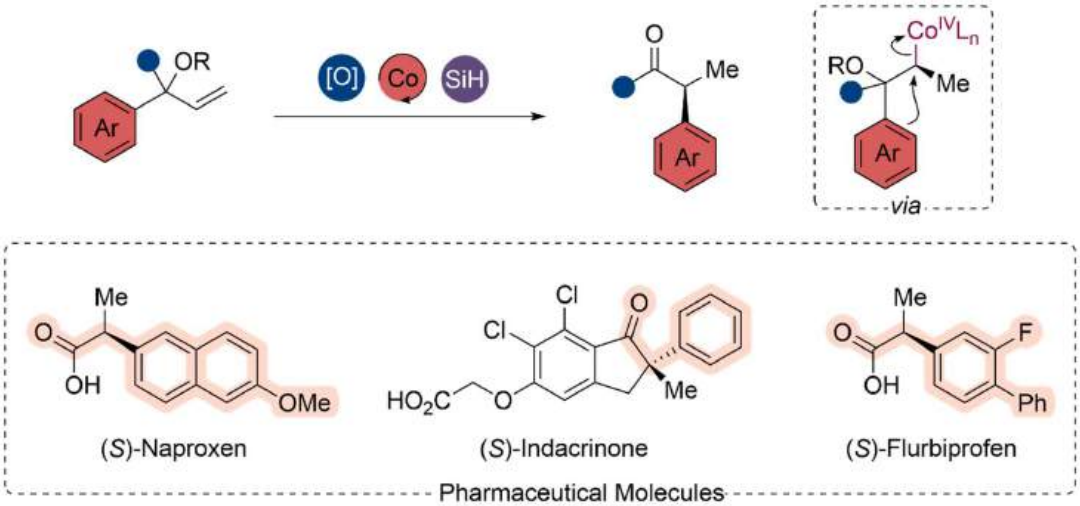
MDR - D2 - O03

Enantioselective synthesis of α-aryl propionyls via a cobalt-catalysed cationic semipinacol rearrangement

Panagiotis G. Kalomenopoulos[1], Balakumar Emayavaramban[1], Nicole K.W X. Tan[1], Craig P. Johnston*[1]
[1]*University of St Andrews, UK*

α-Aryl propionyl compounds constitute pharmaceutical molecules such as the profen series of NSAIDs, which exhibit enhanced bioactivity in particular enantiomeric configurations.[1] Thus, the enantioselective synthesis of this motif has been achieved through the asymmetric transition metal-catalysed couplings or hydrogenations, but these are limited to rare metals and can pose challenges due to pH-related racemisation of tertiary products.[2] An alternative approach is through an enantioselective semipinacol rearrangement through aryl migration, which has been less explored because both allylic alcohol starting materials and products deteriorate under Lewis- or Brønsted-acid conditions, classically needed to generate a carbocation.[3] Cobalt catalysis is an ideal solution as it can implement hydrogen atom transfer and radical–polar crossover events to enable cationic reactivity adjacent to a benzylic alcohol and under much milder reaction conditions.[4] Excellent enantiocontrol is achieved with a chiral cobalt salen catalyst by generating a stereodefined alkylcobalt(IV) species that undergoes invertive displacement *via* 2-electron 1,2-aryl migration.
Mechanistic investigation through internal aryl competition experiments revealed a Hammett *ρ* value of −1.64 with a migratory preference towards electron-rich aromatic rings. This migratory preference elucidates a phenonium cation intermediate, and further mechanistic experiments indicate that a disproportionation reaction between two cobalt(III) salen complexes is responsible for the oxidation to enable this polar reactivity.[5]



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MDR - D2 - O04
Sustainable N-arylation of imidazoles enabled by copper single-atom catalysts

Kaan Karaca[1], Miguel M. de Vries Ibáñez[1], Prof. Gianvito Vilé[1,*]
[1]*Politecnico di Milano, Italy*

The development of sustainable catalysts for C–N bond formation remains a central goal in the pharmaceutical industry, as approximately 80% of marketed drugs contain at least one C–N bond.[1] Traditional Pd-based homogeneous systems, while highly active, suffer from high cost, limited recyclability, and dependence on sophisticated ligands.[2] Attempts to replace Pd with earth-abundant Cu in heterogeneous form have been hindered by ill-defined active sites and inefficient metal utilization in nanoparticle-based catalysts.[3] Copper single-atom catalysts address these limitations by unifying the molecular-level site definition characteristic of homogeneous catalysis with the durability and recyclability of heterogeneous materials, thereby redefining Cu catalysis as a viable alternative to Pd systems for sustainable C–N bond formation. In this work, Cu sites were atomically dispersed on mesoporous graphitic carbon nitride (Cu@mpgCN$_x$) via a hard-template-assisted polymerization method. N_2 physisorption measurements reveal a high specific surface area and well-defined mesoporous structure, while ATR-FTIR and XRD analyses confirm the formation of the graphitic carbon nitride framework. Advanced characterization by XAS and AC-HAADF-STEM verifies the atomically dispersed nature of Cu sites with an average oxidation state close to +1. The combination of ordered porosity and high nitrogen density provides a tailored coordination environment that prevents Cu aggregation while preserving accessible, well-defined active sites. The catalyst achieves 95% yield and 100% selectivity in the N-arylation of imidazole, and was applicable to 15 different N-aryl imidazole derivatives. These results demonstrate that Cu@mpgCN$_x$ represents a new, sustainable and economically viable alternative to traditional Pd-based homogeneous systems for efficient C–N bond formation.

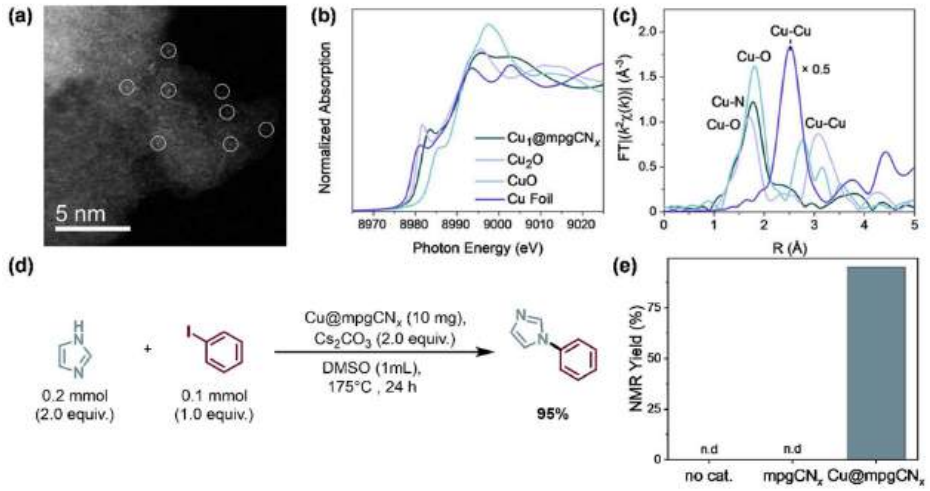

Fig. 2. (a) AC-HAADF-STEM image, (b) XANES, and (c) EXAFS spectra of Cu@mpgCN$_x$. (d) N-arylation of imidazole and (e) representative yields at the selected conditions in (d).

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MDR - D2 - O05
Electrochemical desulfurative borylation of thiols, disulfides, thioethers and thioacetals

Julius Kuzmin[1], Cristiana Margarita[1,2], Johannes Winter[1], Helena Lundberg[1]*
[1]Dept. of Chemistry, KTH Royal Institute of Technology, Stockholm, Sweden; Dept. of Basic and Applied Sciences for Engineering (SBAI), Sapienza University of Rome, Rome, Italy

Low-valent sulfur-containing compounds are abundant among natural and synthetic products, but remain underutilized as starting materials in desulfurative transformations, while sulfoxides, sulfones, and sulfonium salts are more established precursors, for instance in transition metal catalyzed protocols.[1,2] In this work, we present thiols, disulfides and thioethers as precursors in a direct desulfurative electrochemical process for the formation of alkylboronic esters, including late-stage functionalization of pharmaceutically relevant scaffolds and natural products. Alkylboronic acids and esters are a compound class of great importance in organic synthesis, used in powerful transformations such as the Suzuki-Miyaura cross-coupling as well as Chan-Lam couplings.[3-6] We describe the development of a protocol for their synthesis employing pinacol borane (HBpin) under mild electrochemical conditions. The procedure tolerates a wide range of functional groups and is operationally simple as well as scalable, successfully producing gram quantities of borylated product.[7]

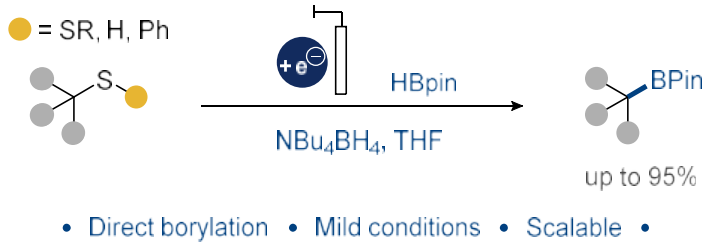

Fig. 1. Electrochemical approach to the synthesis of alkylboronic esters from thiols, disulfides and thioethers.

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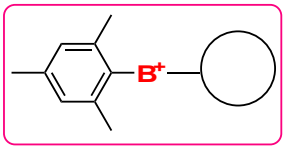
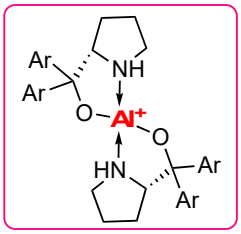
MDR - D2 - O06
Catalytic applications of Di-substituted boron and aluminum cations

Ching-Wen Chiu
National Taiwan University, Taiwan

Group 13 complexes are prototypical Lewis acids with numerous applications in organic synthesis. As the catalytic applications of neutral group 13 catalysts continue to expand, the chemistry of cationic group 13 catalysts has also emerged in recent years. In the past few years, our group has reported that hypercoordinate boron cation ($[Cp^*B\text{-}R]^+$) is effective in catalyzing hydrosilylation and cyanosilylation of carbonyl derivatives.[1,2] Kinetic studies on the related pyridine-coordinate borenium cations revealed that the reagent coordinated boron cation obtained from the reaction between TMSCN and $[Cp^*B\text{-}R]^+$ is much more efficient in promoting the transfer of TMS-CN to the substrate. Subsequently, we discovered that the Cp* substituent is not essential to realize a borinium catalyst. An aryl amino borinium ion, $[TMP\text{-}B\text{-}Mes]^+$,[3] can also catalyze the hydrosilylation of ketones and promote Si-H/Si-C cross metathesis at room temperature.[4] Furthermore, in addition to boron cations, we have prepared a series of prolinol-derived tetra-coordinate chiral aluminum cations, which exhibit considerably higher Lewis acidity compared to $B(C_6F_5)_3$.[5] Our recent studies showed that these aluminum cations are effective in catalyzing the C2-alkylation of indole through asymmetric Michael addition. Theoretical calculations and experimental observations suggest that the amine-aliminum cation cooperative interaction is critical for the activation of C2-H bond. Such synergestic bond activation process can also be extended to the P-H bond of diphenylphosphine oxide for hydrophosphinylation of a,b-unsaturated ketone and amide.





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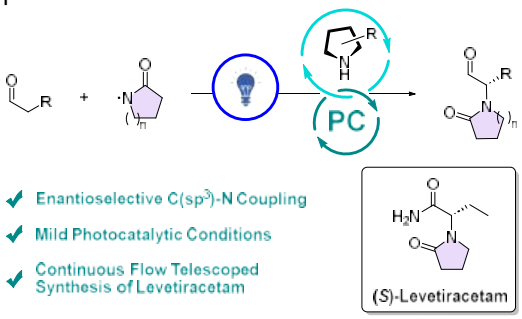
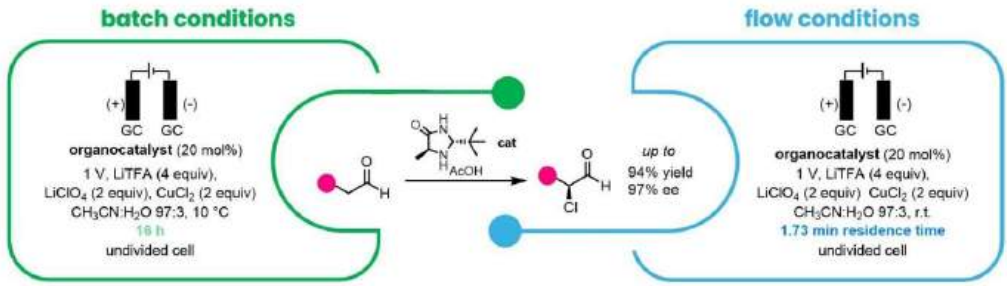
MDR - D2 - O07
Telescoped synthesis of chiral APIs: In flow electrochemical and photoredox catalytic reactions

Maurizio Benaglia
Dipto di Chimica, Università degli Studi di Milano, Italy

Continuous flow technologies, involving the combination of packed-bed and flow reactors, but also CSTR (continuous stirred tank reactors), have allowed to develop telescoped processes aimed to the synthesis of chiral active pharmaceutical ingredients. An efficient continuous flow photoredox reactor was incorporated as one unit of operation into the fully in continuo asymmetric catalytic synthesis of a privileged API.[1] Based on other organophotoredox catalytic transformations involving the generation of N radicals,[2] the telescoped synthesis of the orphan drug, Leviteracetam,[3] and other active pharmaceutical ingredients (unpublished results) have been also developed.
Recent applications of Metallaphotoredox catalysis, the combination of photoredox catalysis with transition metal catalysis, will be also discussed. In particular, a novel synthesis of tryptamine derivatives will be presented.[4]



Finally, the unprecedented, catalytic enantioselective electrochemical alfa-chlorination of aldehydes will be discussed.[5] The reaction was first studied in batch and then further optimised in a continuous flow electrochemical cell to demonstrate the scalability of the process that leads to the formation of the product in >90% e.e. Mechanistic details will be also discussed.



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MDR - D2 - O08
Serendipity results as a driving force for novel reaction development

Serhiy V. Ryabukhin[1,2,3,4], Volodymyr Voloshchuk[1,4], Sergiy Ivonin[4], Dmytro Volochnyuk[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Scientific Research Institute, Ukraine; [4]Institute of Organic Chemistry, NAS of Ukraine

Serendipity results are evidence that accompanies researchers throughout their careers. We, at Enamine, generated more than 90k experimental data per month from our four synthetic departments (Combinatorial Chemistry, Custom Synthesis, Building Block Synthesis, and Process Chemistry). Of course, these results are not only positive. Most of them are regular negative results that are also useful for optimizing reaction conditions, determining scope, diverse chemoinformatic projects, and machine learning. However, nowadays we have begun to put more and more attention to careful analysis of negative results, especially when these negative results are serendipitous with absolutely unexpected reaction pathways.
In this talk, we will show you several examples of such serendipity-based research that led us to discover novel, unpredictable heterocyclizations. Also, we would demonstrate how we found these reactions, detected their pathways, elaborated preparative procedures, and determined their scope and limitations.

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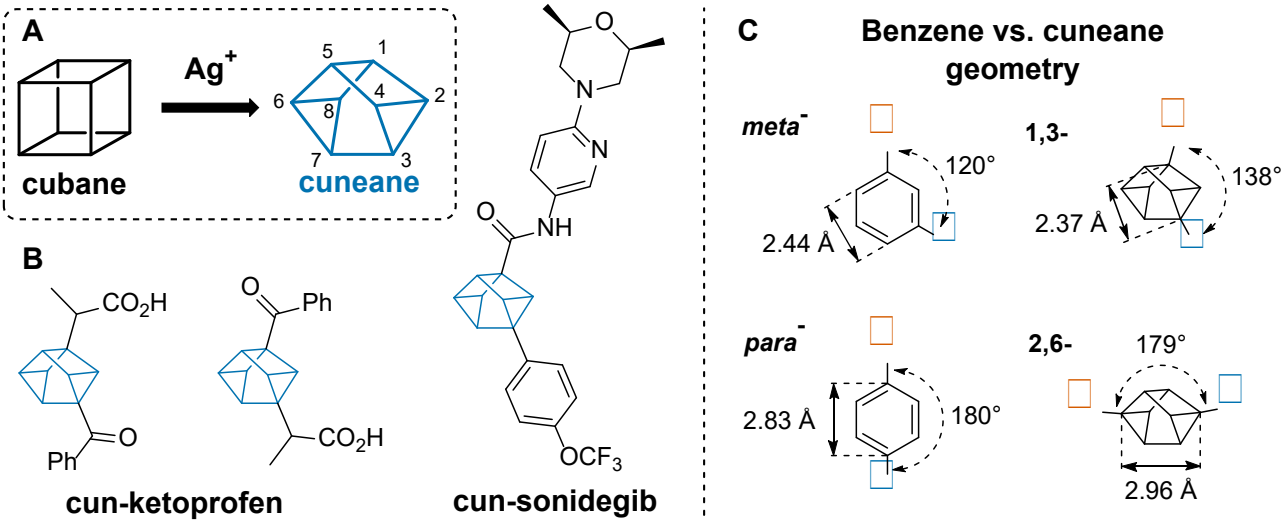
MDR - D2 - O09

Sustainable cubane supply unlocks cuneanes as common tools for medicinal chemistry

Nazar Hryhoriev[1,2], Oleksandr Gaidai[1], Dmytro Volochnyuk[1,2,3,4], Olexandr Pashenko[2,3], Serhiy Ryabukhin[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Scientific Research Institute, Ukraine; [4]Institute of Organic Chemistry, NAS of Ukraine

The value of rigid sp^3-rich benzene mimics for modern medicinal chemistry is well established, yet their routine use depends on whether enabling intermediates can be produced reliably and at scale. For cuneane synthesis, the enabling factor is the availability of cubane. A complicated synthetic protocol that uses custom equipment in the key photochemical step has made key cubane-1,4-dicarboxylate derivatives difficult to access. We address this limitation by implementing a photosensitizer-free, continuous-flow synthesis of cubane-1,4-dicarboxylates on commercial hardware and by converting this capability into preparative access to all three cuneane monocarboxylic acids as well as the 1,3- and 2,6-cuneane acid esters.
The limiting intramolecular photo-[2+2] cycloaddition was redesigned to operate at 365 nm in continuous flow without mercury lamps or sensitizers. Using an MeCN/H_2O/TFA medium and activated-carbon decolorization to suppress UV-absorbing impurities and tubing fouling, the process runs stably over extended campaigns and delivers 54 g h^{-1} productivity. The resulting six-step sequence provides cubane-1,4-dicarboxylic acid monomethyl ester on a multi-hundred-gram scale (25% isolated overall yield), enabling routine preparative availability of the most versatile cubane derivatization handle.
With reliable cubane supply in hand, Ag(I)-catalyzed cubane to cuneane rearrangements were systematically optimized to deliver isomerically pure “para-like” 2,6- and “meta-like” 1,3-cuneane acid-esters on 25 g scale per run. Crucially, we report the first preparative synthesis and isolation of all three cuneane monocarboxylic acids (1-, 2-, and 3- on 3 to 20 g scale). Together, these advances “upgrade” cuneanes from milligram curiosities into practical, scalable sp^3-rich building blocks for medicinal chemistry.



A: Cubane isomerization to cuneane; **B**: Literature examples of the cuneane-based drug analogues;
C: Geometry comparison of meta- and para-substituted benzenes to the 1,3- and 2,6- disubstituted cuneanes.

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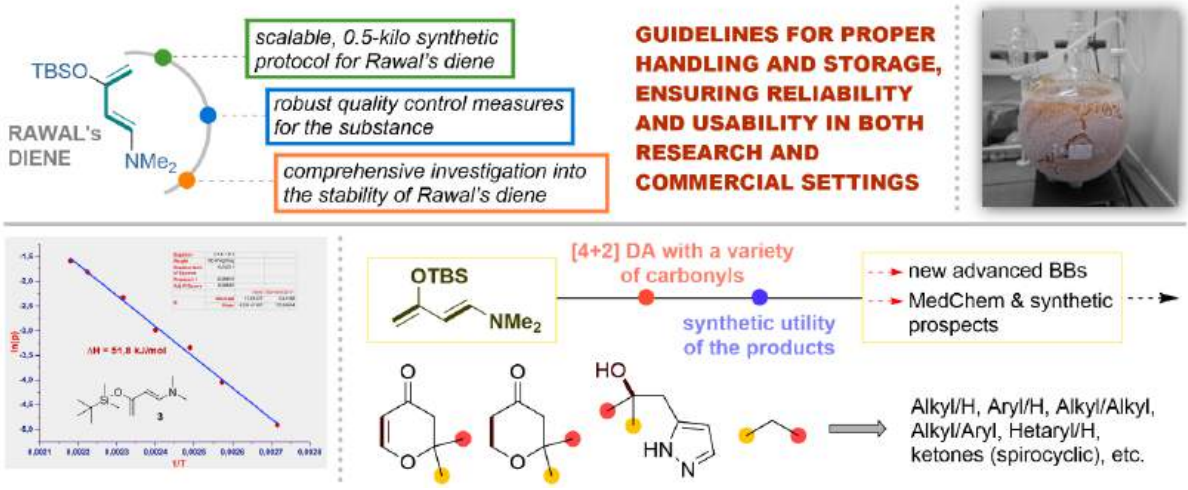
DOI: 10.26434/chemrxiv-2025-3fhx3

MDR - D2 - O10
Turning a bottleneck into a tool: Rawal's diene case

Oleksii Shamrai[1], Eugeniy Ostapchuk[1,2], Dmytro Leha[2,3], Dmytro Volochnyuk[1,2,3,4], Serhiy Ryabukhin[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Scientific Research Institute, Ukraine; [4]Institute of Organic Chemistry, NAS of Ukraine

Electron-rich dienes have transformed modern cycloaddition chemistry by enabling rapid access to densely functionalized heterocycles, particularly through hetero-Diels-Alder reactivity. Within this class, Rawal's diene, a distinctive enamine/enol ether hybrid, has become a powerful second-generation reagent that frequently outperforms well-established Danishefsky's diene in reactions with carbonyl electrophiles, offering enhanced reactivity and synthetic flexibility. Paradoxically, despite its outstanding performance, Rawal's diene has remained underutilized. Its broader implementation has been limited not by conceptual value, but by practical barriers – restricted commercial availability, uncertain storage behavior, incomplete stability profiling, and the lack of a truly scalable, reproducible synthesis suitable for routine laboratory use.
In this report, we address these limitations in a comprehensive and application-oriented manner. A robust two-step protocol was developed and validated, enabling the reliable multigram preparation of Rawal's diene on a scale of over 0.5 kilos per run, with high purity and reproducibility.
Beyond synthesis, we provide a detailed assessment of the stability profile of Rawal's diene and introduce improved quality control workflows.
Finally, the synthetic value of the reagent was illustrated through hetero-Diels-Alder cycloadditions with a diverse set of aldehydes and ketones, followed by representative downstream derivatizations of the products.
Collectively, this study converts Rawal's diene from a "high-potential but inconvenient" reagent into a practical and scalable tool, expanding its accessibility and strengthening its role in contemporary synthetic chemistry.



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MDR - D2 - O11

Highly stereoselective synthesis of bioisosteric fluorinated 3-azabicyclo[3.1.0]hexane scaffolds via asymmetric cu catalysed (3+2) cycloadditions

Paul A. Nolan, Adam R. Daly, Julia Bruno-Colmenarez, Patrick J. Guiry
University College Dublin, Ireland

The incorporation of bioisosteric motifs into APIs has become a common strategy to try to improve the pharmacokinetic and pharmacodynamic properties of their parent compounds.[1,2] This success is linked to the introduction of more topologically rich bicyclic systems.[3] Aza-bicyclo[3.1.0]hexanes are a notable success of this strategy with these bicyclic motifs featuring in boceprevir[4] and nirmatrelvir[5]. Additionally, fluorine incorporation has become increasingly attractive for its relatively small size, increased lipophilicity and marked resistance to metabolism.[6] Difluorinated analogues of the gem-dimethyl aza-bicyclo[3.1.0]hexane analogues would be of interest for the advantages that fluorine offers. However, difluorinated analogues remain absent due to the difficulty in accessing fluorinated compounds. Without a general and highly stereoselective method to access these scaffolds, their use as molecular building blocks in combinatorial chemistry for the rapid development of drug libraries is severely impeded.
Many methods exist for the synthesis of 3-azabicyclo[3.1.0]hexane scaffolds[8-12] but emphasis has been placed on the (3+2) cycloaddition of substituted cyclopropenes with azomethine ylides to generate these ring systems.[13-16]

As part of our group's ongoing interest into asymmetric metal-catalysed (3+2) cycloadditions,[17] we report the development of a general, high yielding and highly stereoselective synthesis of new fluorine-containing azabicyclo[3.1.0]hexanes via the first asymmetric metal-catalysed (3+2) cycloaddition of azomethine ylides with fluorinated cyclopropenes. 20 novel fluorinated azabicyclo[3.1.0]hexanes have been synthesised in excellent yields of up to 97%, >20:1 exo/endo ratio and up to 98% ee that showcase this methods generality and adaptability. We have shown the methods amenability to late stage functionalisation and the synthetic utility and viability of these as chiral molecular building blocks through scale-up and a variety of derivatisations to prepare complex biologically relevant motifs. Additionally, mechanistic experiments and DFT calculations have been carried out that support a new mechanism for this 3+2 cycloaddition that exploits the unique reactivity of fluorinated cyclopropenes.

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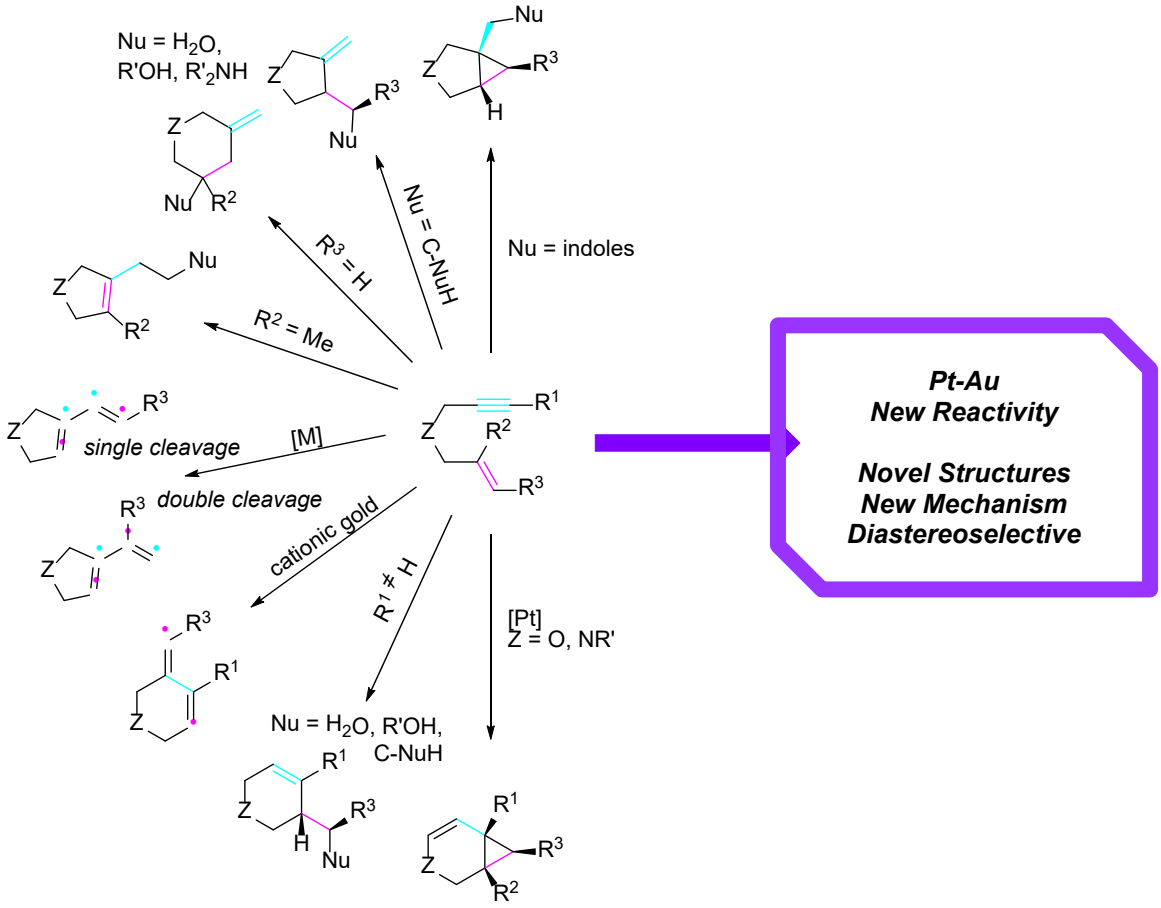
MDR - D2 - O12
Expanding drug-relevant chemical space through Pt-Au bimetallic catalysis

Khaleel Zareen, María Paz Muñoz-Herranz
Lancaster University, UK

Bimetallic catalysis has evolved in recent years as a powerful strategy towards the synthesis of new structures, inaccessible through monometallic systems. Homogeneous Pt-Au bimetallic catalysis has scarcely been reported on, except for by Muñoz and co-workers,[1,2] to achieve novel, azole-containing compounds with promising antimicrobial activity.[3] The key to the enhanced and divergent reactivity established here is due to the highly electrophilic bimetallic carbene intermediate,[4] and, thus, applying this new methodology to known systems that proceed via a gold carbene intermediate should unlock new possibilities. 1,6-Enynes have been known to undergo several different reactions, including the nucleophilic addition of indoles.[5-7] Under Pt-Au bimetallic catalysis, new interactions with 1,6-enynes have been discovered to give divergent reactivity to access new structures diastereoselectively.



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MDR - D2 - O13

Replica Exchange with Flexible Timing (REFT): a novel replica exchange variant for efficient conformational sampling and free energy calculations

Fardine Ameli, Yvan Vander Heyden, Debby Mangelings, Kenno Vanommeslaeghe
Vrije Universiteit Brussel (VUB), Faculty of Medicine and Pharmacy, Research group Analytical Chemistry, Applied Chemometrics and Molecular Modelling, Brussels, Belgium.

Molecular dynamics (MD) simulations are routinely used to study the atomistic behavior of molecular systems. Unfortunately, conventional MD simulations often struggle to sample the full conformational space associated with the process of interest, as the required timescales commonly exceed practical computational limits. To overcome this, enhanced sampling techniques, such as replica exchange MD (REMD), have gained popularity because of their capability to accelerate free-energy barrier crossing and enrich configurational sampling. Over the past decade, numerous REMD variants have emerged, including multi-dimensional exchange schemes and hybrid approaches. The proliferation of these variants reflects the diversity of molecular systems (from small peptides to larger macromolecules) and the continued drive to improve sampling efficiency while rigorously preserving the correct target ensemble [1-4].

REMD runs multiple replicas of the system in parallel (e.g., different temperatures or Hamiltonians) and exchanges the conformations among them at fixed intervals. This exchange reduces correlation times and improves sampling efficiency by allowing the system to overcome kinetic barriers through transitions into neighboring states with lower barriers. Effective REMD requires moderate overlap in configurational space between neighboring replicas to facilitate efficient exchanges. Therefore, traditional REMD often demands a large number of closely spaced replicas to achieve optimal exchange rates, partially negating its computational advantage.

Here, we introduce Replica Exchange with Flexible Timing (REFT), a novel REMD variant that decouples exchange attempts from the fixed exchange time by permitting exchanges between adjacent replicas at variable, earlier time points relative to the scheduled exchange evaluation. This flexible timing elevates exchange rates and thereby reduces the computational cost for obtaining a given amount of sampling. While we conceived this novel approach for the purpose of calculating adsorption free energies for disordered adsorbants, we demonstrate the method's validity by obtaining accurate solvation free energies for small molecules and sampling the conformational ensembles of short peptides.

This work was supported by the Research Foundation Flanders (FWO) (project number G015022N). The supercomputing resources and services used in this work were provided by the VUB and the VSC (Flemish Supercomputer Center, project 2025_078), the latter being funded by the FWO and the Flemish Government.

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MDR - D2 - O14
Diastereoselective access to α-hydroxy-lactams through carbene-carbonyl cyclization

Agathe Fayolle[1], Claude Spino[1], Léo Schitter[2]
[1]Université de Sherbrooke, Canada; [2]Université de Strasbourg, France

Nitrogen-containing heterocycles are ubiquitous structural motifs in pharmaceuticals due to the broad range of biological activities they confer to molecules. Among them, α-hydroxy-γ-lactams stand out as valuable synthons found in natural products and therapeutic agents exhibiting antifungal, anti-HIV, anti-dementia, and cytotoxic activities. Despite their importance, synthetic methods specifically targeting α-hydroxy-γ-lactams remain limited, as existing approaches often rely on structurally complex starting materials, exhibit narrow substrate scope, or provide limited stereochemical control.
N-Heterocyclic carbenes (NHCs) are nucleophilic species due to the strong electron-donating nitrogen atoms adjacent to the divalent carbene carbon. Previous studies have demonstrated that NHCs can be generated from imidazole derivatives and react with different carbonyl substrates. However, intramolecular NHC–carbonyl additions have rarely been reported, likely due to the instability of the resulting cyclized intermediates. Herein, we report a concise and efficient three-steps strategy for the diastereoselective synthesis of α-hydroxy-γ-lactams based on an NHC–carbonyl cyclization followed by ozonolysis and deformylation. Notably, the method enables the stereocontrolled formation of a quaternary carbon center, a longstanding challenge in lactam synthesis. A wide variety of substituents can be introduced from readily accessible enones or γ-haloketones, providing a concise, operationally straightforward entry into structurally diverse and biologically relevant α-hydroxy-γ-lactams.

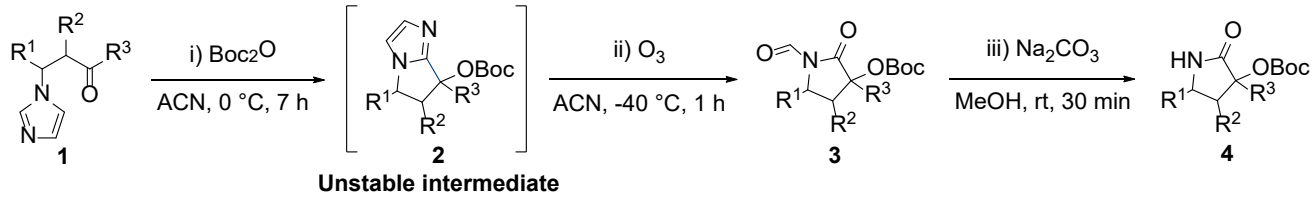


Fig.1. Formation of a Lactam by Intramolecular Addition of a NHC to a Ketone.

MDR - D2 - O15

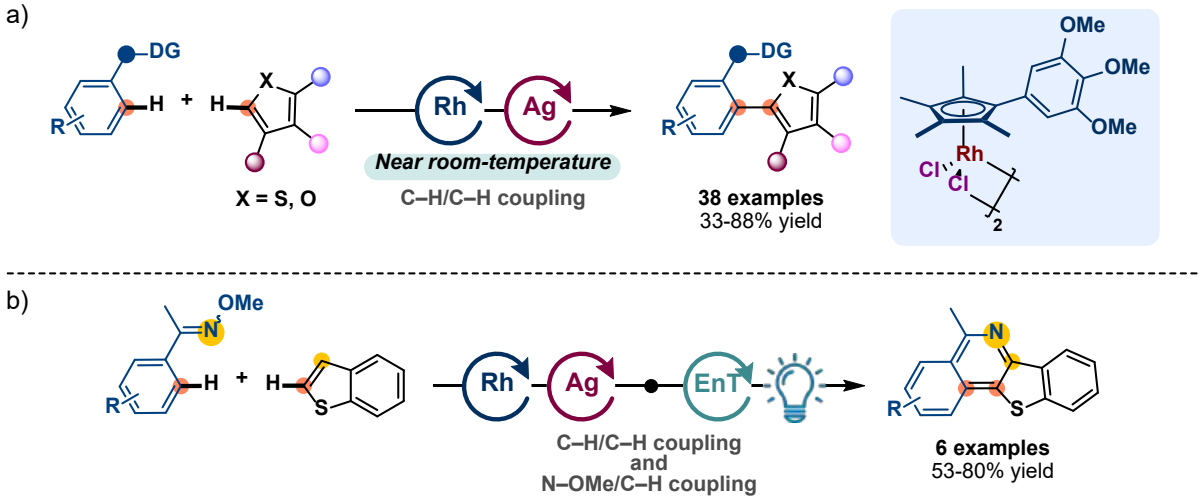
Rh(III)-catalyzed room-temperature heterobiaryl synthesis: Elucidating the complementary roles of Cp-ligand design and Ag(I) salts

Laura Thirion[1], Marie Peng[2], Sarah Gomes[1], Jean-François Soulé[1]
[1]Chimie ParisTech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, France; [2]ISCR - Institut des Sciences Chimiques de Rennes, France

Aryl-thiophenes and related arylheteroarenes are privileged motifs in pharmaceuticals and organic electronics. Their classical synthesis relies on cross-coupling of prefunctionalized partners. More recently, direct C–H bond arylation has improved step economy, but the ideal is cross-dehydrogenative coupling (CDC), which forges a C–C bond directly from two C–H bonds with ≈98% atom economy (*H_2 only as side-product*).[1] However, room-temperature (RT) CDCs remain elusive: current methods require 100–160 °C. Developing true RT conditions would improve functional-group tolerance and lower energy use, making CDCs more appealing for scalable process chemistry.

In this work, through rational design and combined experimental/computational mechanistic studies, we enable **RT-CDC** between heteroarenes and arenes *via* two advances: (*i*) an electron-rich, anisosteric Cp–Rh(III) catalyst that promotes selective *ortho*-C–H bond activation of arenes,[2] and (ii) Ag(I) acting as a catalyst for heteroarene C–H bond activation, beyond its usual role as a terminal oxidant.[3] This catalytic system shows broad scope, high regioselectivity, and functional-group tolerance (including halides), offering a sustainable route to heterobiaryls for pharmaceuticals and organic electronics and showcasing ligand/coinage-metal co-design to lower the thermal barrier.

Additionally, when combined with a metal-free, room-temperature photocatalytic energy-transfer cyclization, this method provides direct access to pyridine-containing π-fused tetracyclic scaffolds, opening the door to further optoelectronic applications.



Scheme 1. a) General scheme for the Cp-Rh(III)/Ag(I)-catalyzed RT-CDC of arenes and heteroarenes. b) Tandem Cp-Rh(III)/Ag(I)-catalyzed RT-CDC and Photocatalyzed Energy Transfer cyclization for pyridine-containing π-fused tetracyclic scaffolds synthesis.

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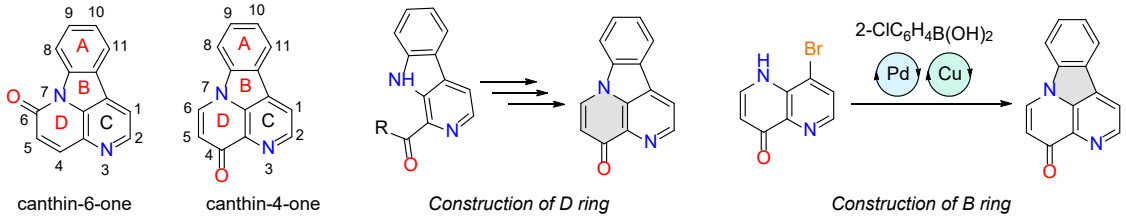
MDR - D2 - O16
Synthesis of canthin-4-ones and related molecules

Maria Koyioni[1], Panayiotis A. Koutentis[2]
[1]Dept. of Chemistry, National and Kapodistrian University of Athens, Greece; [2]Dept. of Chemistry, University of Cyprus, Nicosia, Cyprus

Canthinones are a subgroup of β-carboline alkaloids, represented by canthin-6-ones and canthin-4-ones. More than 40 natural analogues of canthin-6-ones have been isolated to date, but only three natural canthin-4-ones: tuboflavine, norisotuboflavine, and isotuboflavine have been reported. While scarce, both natural and synthetic canthin-4-ones, have potential in medicinal chemistry as they exhibit antimicrobial and phosphodiesterase-inhibitory activities. Access to diverse libraries of canthin-4-ones for structure-activity relationship studies remains limited owing to the lack of reliable general syntheses. Early and recent routes to canthin-4-ones, are based on β-carboline precursors, proceeding via construction of the D-ring, thus diversification of the carboline backbone is limited. Herein, we describe a short synthesis of canthin-4-ones, and isocathin-4-ones, via construction of the B-ring which enables, facile diversification of the A ring.[1] Additionally, further unexpected products arising from this chemistry and their efficient synthesis will be discussed.



The authors thank the Research and Innovation Foundation for funding (POST-DOC/0718/0005).

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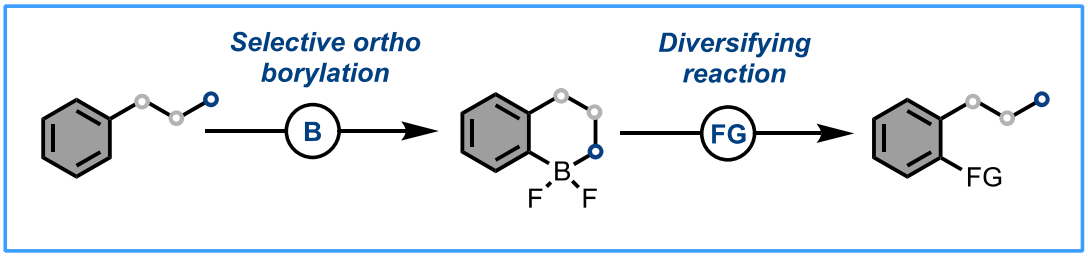
MDR - D2 - O17

Selective boron-based *ortho*-directed functionalization strategies of aromatic substances



A series of highly efficient, regioselective methods for the functionalization of 2-aryl-heteroarenes1-3 and N-aryl amides4 has been developed, leveraging the unique reactivity of boracycles. These strategies enable installation of diverse functional groups, including halogens (chloro, bromo, iodo), hydroxyl, amine, BF_2, and aryl groups, with exceptional ortho site-selectivity and broad substrate scope. Collectively, these methods underscore the synthetic utility of boracycles in enabling precise, scalable, and operationally simple transformations, with significant applications in medicinal chemistry and materials science.

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MDR - D2 - O18
Direct active template synthesis of cyclic peptide catenanes

Karen Junghans[1,2], Julia Szymanska[3], Zhe Li[1,2], Emma L. Wadforth[1,2], Ellen M. G. Jamieson[1,2], Yew Mun Yip[1], Stephen M. Goldup[3], Charlie T. McTernan[1,2]
[1]Artificial Molecular Machinery Laboratory, The Francis Crick Institute, UK; [2]Dept. of Chemistry, King's College London, UK; [3]School of Chemistry, University of Birmingham, UK; [4]Chemical Biology Science and Technology Platform, UK

Cyclic peptides are an emerging therapeutic modality bridging small molecules and biologics, with antimicrobial, anticancer, and antiviral properties.[1] Cyclisation restricts conformational freedom and can enhance binding to targets.[2] However, cyclic peptides often show poor proteolytic stability and cell permeability, limiting their use to extracellular targets.[3] Synthesising mechanically interlocked molecules in which one of the components is a cyclic peptide is a longstanding challenge in synthetic supramolecular chemistry, inspired in no small part by the intriguing biological properties of lasso peptides, which contain this motif. However, to date, reported methods to access interlocked cyclic peptides make use of highly engineered polyproline macrocycles with non-peptide linear partners, as cyclic peptides more generally are poor hosts for either active or passive template mechanical bond forming methodologies. Unfortunately, even in these optimised cases the yields obtained are typically low and the cyclic peptide component has minimal structural diversity. Here, we show that reversing this standard strategy, by forming the peptide macrocycle in the mechanical bond forming step itself using an active template reaction, is a general solution to the synthesis of cyclic peptide catenanes. Furthermore, we show that the mechanical bond controls the conformational flexibility of the cyclic peptide, enhances its stability to proteolysis, and modulates its lipophilicity, all key parameters for biological applications. Our approach thus opens the way to mechanically engineering the properties of biologically relevant cyclic peptides.

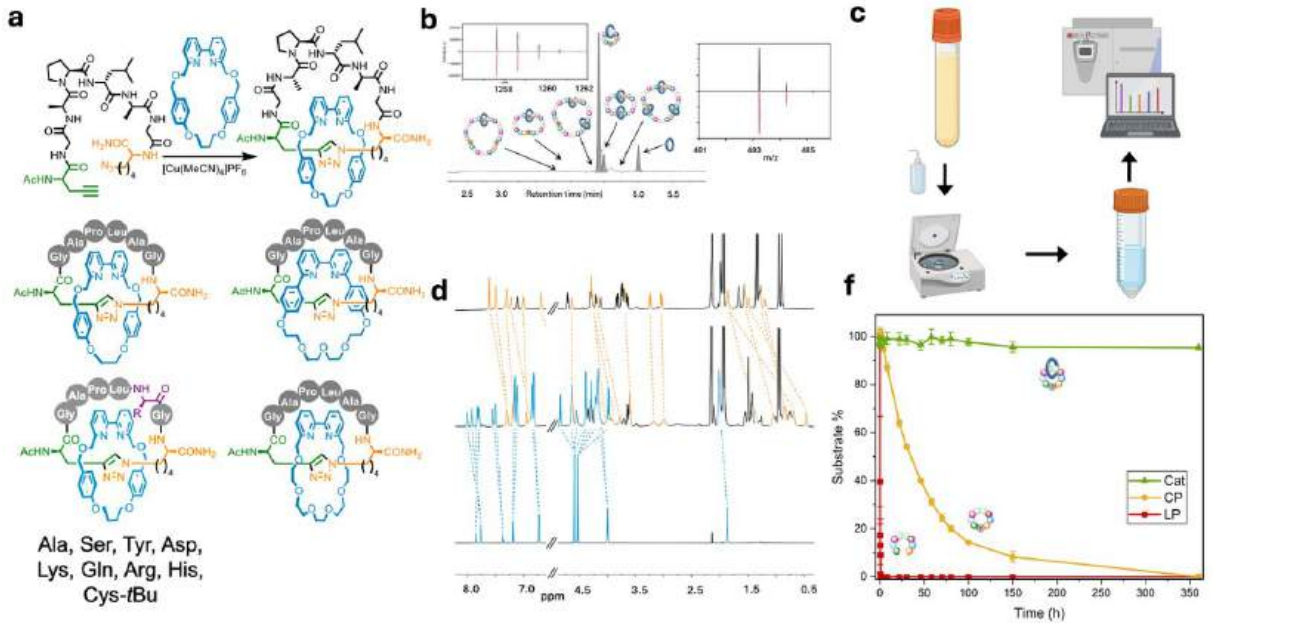

Fig. 1. a. Synthesis and exemplar scope of Cyclic Peptide Catenanes using Active Metal Template. **b**. LCMS and HRMS of crude reaction mixture, showing desired [2]catenane and oligomeric products. **c.** Schematic of plasma stability experiment workflow. **d.** Stackplot of catenation, with cyclic peptide top, catenane middle, and bipyridine macrocycle bottom, confirming interlocked structure. **e.** Plasma stability experiments, showing degradation of linear and cyclic peptides, whilst the mechanically interlocked peptide remains stable over >360 hr in mouse plasma at 37 °C.

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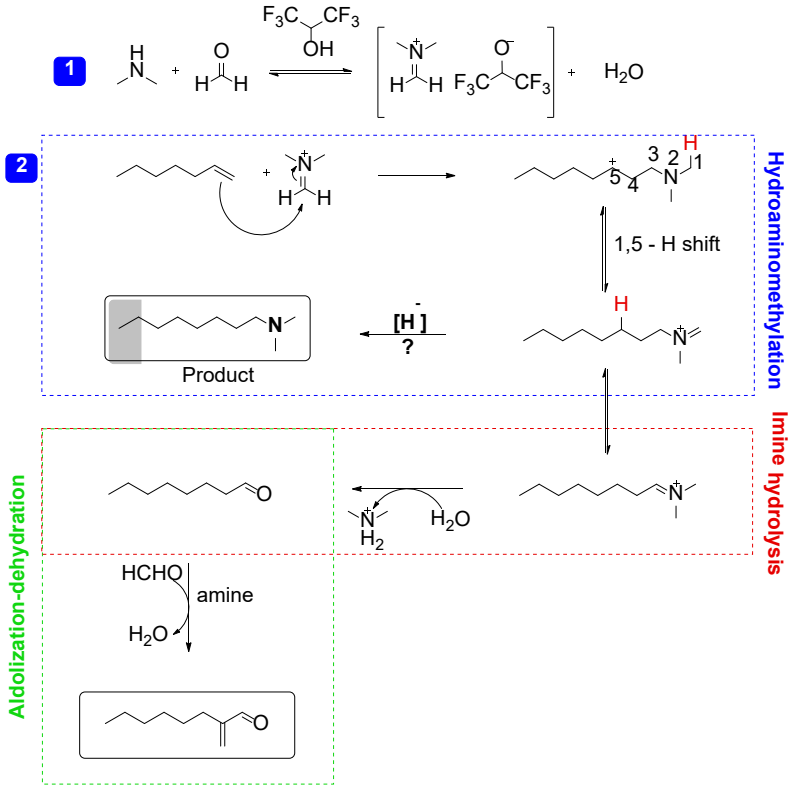
MDR - D2 - O19
A metal-free iminium-driven synthesis of amines from alkenes

Gibrael Fadel, Karine De Oliveira Vigier, François Jérôme
IC2MP, Institut de Chimie des Milieux et Matériaux de Poitiers, France

The synthesis of tertiary amines from alkenes according to literature follows three major chemical genres: hydroamination, hydroaminomethylation, and hydroaminoalkylation[1]. The use of both homogeneous and heterogeneous catalysts encompasses these families and has been indispensable for ensuring the success of such approaches. There are various drawbacks for these approaches including thermodynamic limitations, selectivity issues, and issues dealing with the synthesis, stability and recyclability of the catalysts. Till now, few metal-free approaches have been investigated[2], and even fewer approaches are considered environmentally benign.
Here, we propose a novel metal-free approach based on a previous study done in our group targeting the synthesis of α,β unsaturated aldehydes[3]. The approach aims to trap a highly electrophilic reaction intermediate using formic acid as reductant, thus favoring a hydroaminomethylation style reaction leading to the production of antimarkovnikov addition products, exclusively, thanks to 1,1,1,3,3,3-hexafluoroisopropanol (HFIP) the ideal solvent. The reaction ideally functions at low temperature for activated and non-activated alkenes, *via* an *in situ* formed Eschenmoser's salt formed thanks to the dialkylamine and *p*-formaldehyde used. Generally, the reactions' durations depend heavily on the type of alkenes used with a time scale ranging from few hours to several days. On one hand, terminal alkenes and cyclic alkenes excel this transformation, unlike internal linear alkenes, on the other hand, which show either a low reactivity towards the reduction reaction by formic acid or a total inactivity. Among the linear terminal and cyclic alkenes that have been tested, the selectivity for the tertiary amine ranges between 53% and 90%, whereas for cis and trans internal linear alkenes a low selectivity of around 10% was observed. Ideal reaction conditions along with mechanisms explaining this type of transformation will be presented.



Scheme. A simplified reaction scheme showing the general mechanism and the research objective.

Acknowledgements: The authors are grateful to PEPR SPLEEN, ECOCHEM project for the financial support.

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MDR - D2 - O20
Using photoswitchable imines to drive (dark)transimination reactions uphill

Jake L. Greenfield[1,2]
[1]School of Chemistry, University of St Andrews, UK; [2]Institut für Organische Chemie, Universität Würzburg, Germany

Molecules and materials comprised of dynamic-covalent imine bonds display many desirable properties, including stimuli-responsiveness, recyclability, and effortless preparation, among others. However, the *E*/*Z* photochromism of imines has often been overlooked due to historically poor performance compared to other photoswitches, typically showing less than 50% conversion to the metastable state and thermal half-lives of under one minute.[1] Recently, we developed a strategy that significantly improves these photoswitching properties, achieving quantitative *E*-to-*Z* conversion with visible light and extending the thermal half-lives of the metastable *Z*-state to over one day.[2,3] We further found that the regiochemistry of the C=N bond plays a significant role in the switching behavior.[3,4] Through a systematic investigation, a set of design rules for this novel class of imine photoswitch has now been reported.[5]
With these improved photoswitching properties, we explored the light-dependent dynamic-covalent chemistry of these photoswitches. We found that they can drive transimination reactions energetically uphill when irradiated with light,[6] operating via a mechanism akin to a light-driven information ratchet.[7] Moreover, a non-photoresponsive transimination could be driven out-of-equilibrium by coupling it to the photoresponsive transimination reaction.[8] This talk provides an overview of our recent work.[9]

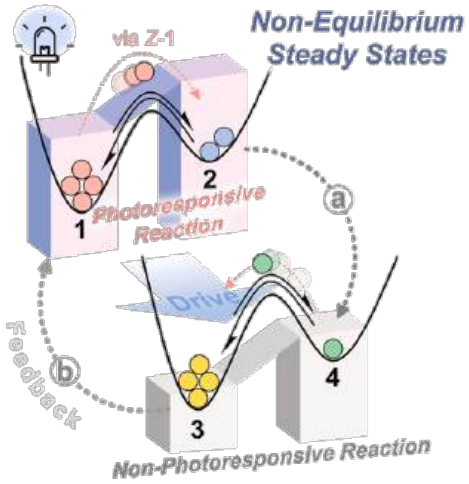

Fig. 1. Schematic of the coupling of a light-driven transimination reaction to a non-photoresponsive transimination reaction.

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MDR - D2 - O21

A Plausible Model for Tightly Bound Single Metal Atoms on Carbon Nitride for Computational Studies on Single Atom Catalysis.

Maria Voccia[1], Sergio Tosoni*[1]
[1]Dept. of Materials Science, University of Milan-Bicocca, Via Roberto Cozzi 55, 20125, Milan, Italy

The development of more sustainable and efficient methodologies for the catalytic synthesis of biaryl derivatives is a central topic in organic chemistry, due to their widespread occurrence as key motifs in pharmaceuticals, agrochemicals, and advanced materials.[1] The dehalogenation and the iodine recovery of aromatic organic compound is also a topic of high environmental relevance. As reported in literature, the Ullmann homocoupling reaction can be obtained using homogeneous catalytic protocols,[2] that could lead to deactivation or difficulties in recovery and reuse of catalyst and contamination from residual metals, compromising their high efficiency. The alternative application of heterogeneous catalysts offers enhanced stability and recyclability, however, introduces challenges as reduced activity, harsh reaction conditions or protracted reaction times.[3]

In this context, single-atom catalysts have emerged as a solution by isolating individual metal atoms on solid supports. Our group have developed a family of TM-based SACs[4-5] supported on mesoporous graphitic carbon nitride. An alternative model of single metal atoms stably bound to a carbon nitride matrix—a widely studied paradigm for SACs — is employed in this study.

These materials have been applied as photocatalysts for the Ullmann homocoupling of aryl halides under ambient conditions and visible-light irradiation, enabling milder and more sustainable reaction conditions than previously reported. Recent experimental results from the group of Gianvito Vilé (Politecnico di Milano), complemented by spectroscopic measurements performed by Lorenzo Mino (University of Torino), highlight the high efficiency of SACs in C–C coupling reactions of aryl halides.

Here, through an in-depth DFT study, the mechanism of the Ullmann C–C coupling reaction mediated by SACs is investigated, elucidating the role of the isolated metal atom and the effect of visible-light irradiation.[6]

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MDR - D2 - F01
Synthesis of bispidine-based fluorinated chemosensors for selective analytes recognition

Giulia Marcolli[1,2], Paola Scampini[1], Sara Camorali[1], Arianna Rossetti[1,2], Massimo Cametti[1], Alessandro Sacchetti[1,2]
[1]Politecnico di Milano, Italy; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy

One of the major challenges in medical, environmental and pharmaceutical fields is the reliable and specific detection of analytes in complex mixtures. Proton Nuclear Magnetic Resonance (^{1}H-NMR) is a powerful analytical technique often employed to tackle it, able to reveal molecular organization and atomic-level structure. However, its interpretation in complex mixtures can be challenging due to the complexity of spectra caused by signal overlapping and low selectivity[1]. To overcome this issue, chemosensing systems use specific molecular interactions to generate simplified, distinguishable signals, enabling simultaneous detection of multiple species[2].
In this context, **^{19}**F-labeled molecular probes represent a powerful tool, as they generate unique ^{19}F-NMR signals with minimal background interference[1]. In this work, bispidines, heterocyclic compounds consisting of two fused piperidine rings, were selected as a scaffold for metal chelation thanks to their rigid framework, conformational adaptability and multiple nitrogen donor atoms. During synthesis, Mannich reaction was employed to selectively introduce both ^{19}F-labelled moieties (such as F, CF_3 and OCF_3) and additional nitrogen atoms to enhance coordination. With this procedure, two types of scaffolds were prepared: bidentate bispidines via a one-pot reaction, and tetradentate bispidines via a multi-step process. These compounds were fully characterized and tested to evaluate their ability to form coordination complexes with different metal salts. The most promising molecules were tested for organic molecule recognition in solution, studies of coordination competition between different metal salts and evaluation of ligand extraction capacity with two-phase mixtures. Thanks to the simplicity of ^{19}F-NMR spectrum, it was possible to study all chemical shifts induced by coordination and correlate them directly to specific bispidine-metal complexes or complex-organic molecule, allowing rapid identification of the bound species.

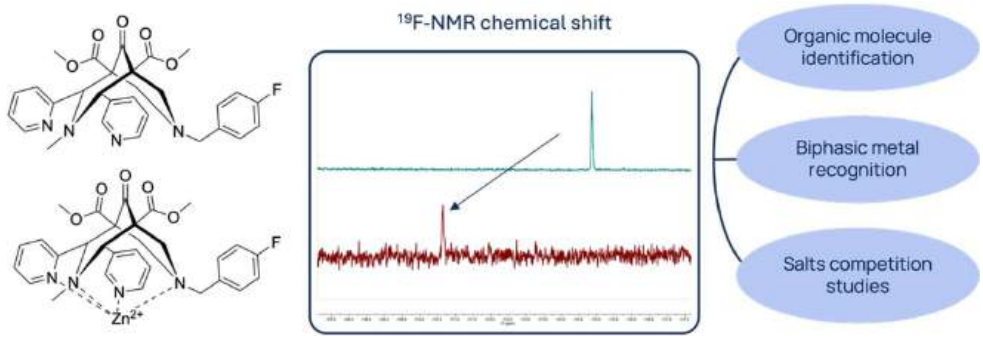

Fig. 1. Graphical abstract

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MDR - D2 - F02

The two-dimensional locksmith: Ligand-driven structural changes in self-assembled supramolecular networks of bisporphyrin cages at the solid-liquid interface

Navathej Preetha Genesh[1], A. Priscila Gia[2], Alberto de Juan[2], Alberto de Juan[2], Miguel García-Iglesias[3], David González-Rodríguez[2], Kuanl S. Mali[1], Steven De Feyter[1]
[1]KU Leuven, Belgium; [2]Universidad Autónoma de Madrid, Spain; [3]Universidad de Cantabria, Spain

Rational control over two-dimensional molecular self-assembly on surfaces is fundamental to designing advanced functional materials.[1] Central to this goal is the design and manipulation of supramolecular interactions that direct molecular organization at interfaces. Shape-persistent organic cages have distinguished themselves as robust, versatile building blocks for constructing ordered networks through bottom-up fabrication.[2] Their fixed structural geometry, coupled with their capacity for host–guest recognition and site-specific ligand coordination, makes them especially valuable for applications requiring precise spatial organization and dynamic tunability. While the behaviour of these cages has been studied extensively in solution, achieving molecular-level understanding of their assembly kinetics and structure at interfaces remains elusive. This presentation details the scanning tunnelling microscopy (STM) investigation of cofacial (Zn^{II})bisporphyrin cages[3] at the solid-liquid interface, providing real-space, submolecular visualization of their packing motifs and dynamic changes. We employed distinct ligand complexation methods, both inside the internal cavity and coordinating externally, to structurally modulate the resulting cage assemblies at the interface. This study of surface-confined organization of cages yields molecular insights into their packing behavior and adaptability, paving the way for interface-driven functional materials.

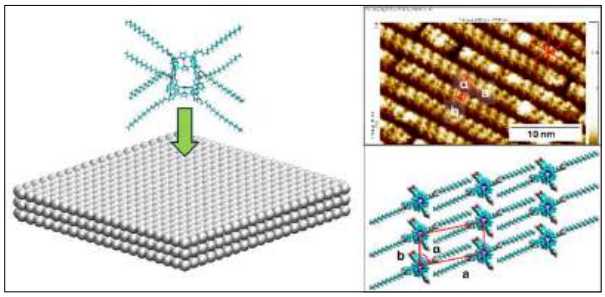

Fig. 2. Interfacial self-assembly of cofacial (Zn^{II}) bisporhyrin cages and their molecular resolution using STM.

Acknowledgements: Financial support is acknowledged from KU Leuven–Internal Funds (C14/23/090), and the FWO and F.R.S.-FNRS Excellence of Science (EOS) program (FWO G0H2122N).

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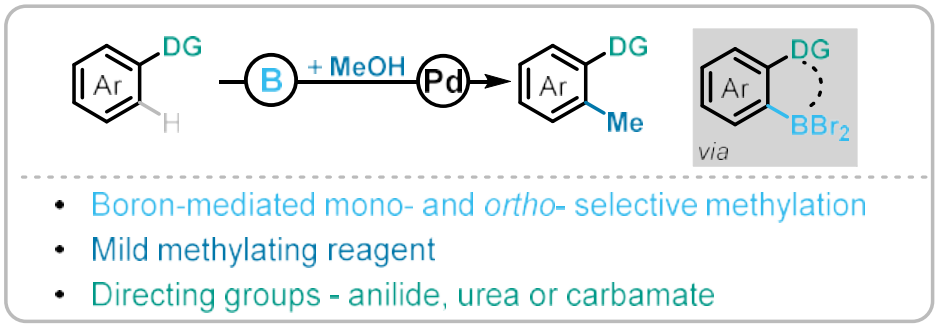
MDR - D2 - F03

Boracycle-mediated aromatic C-H *ortho*-methylation using methanol as a methylating reagent

Vincent Nilsson[1], Ganesh Shinde[1], Daniele Antermite[2], Henrik Sundén[1,2]
[1]University of Gothenburg, Sweden; [2]AstraZeneca, Sweden



The "magic methyl effect" plays a crucial role in medicinal chemistry, enhancing the biological activity of compounds through the introduction of methyl groups.[1] Recognizing its significance, we focused on developing a methylating reaction capable of late-stage functionalization. Our research leverages a BBr_3-mediated borylation, which employs a chelating functional group on an aromatic system to selectively form a boracycle at the *ortho*-position.[2,3] Previously, we demonstrated that this boracycle is an effective participant in Suzuki-Miyaura couplings for arylation and benzylation.[4,5] Building on this work, we have now developed boracycle-mediated methylation, using methanol as an innovative methyl source.

We have shown that this boracycle-mediated methylation reaction effectively provides the *ortho*-methylated product of substrates with anilide, urea, and carbamate directing groups. By developing a method for high-throughput experimentation with this reaction, we have been able to thoroughly investigate its parameters and robustness. The reaction demonstrates good functional group tolerance, facilitating product formation even in the presence of various functional group additives. As we continue to investigate the reactions applicability for late-stage functionalization, we anticipate that this approach will contribute meaningfully to the tools available for organic synthesis, offering practical solutions for the selective functionalization of complex molecules.

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MDR - D2 - F04

Innovative scaffolds based on 4-hydroxyproline as chemical permeation enhancers, for transdermal drug delivery

Bárbara Sampaio[1], M. Luísa C. Do Vale[1]
[1]LAQV-REQUIMTE, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Porto, Portugal

Transdermal drug delivery systems (TDDS) offer numerous advantages over traditional oral and parenteral administration, which often suffer from poor absorption and metabolic degradation. TDDS enable simple administration and provide a sustained drug release, which results in uniform plasma drug levels. Yet, effective delivery through the skin remains challenging because the *stratum corneum*- the skin´s outermost layer- acts as an effective barrier to many therapeutic molecules. One of the methodologies developed to overcome this limitation consists in the use of chemical permeation enhancers (CPEs). Among these, amino-acid based CPEs stand out as a particularly promising class, offering biocompatibility, low cytotoxicity and reversibility of action [1],[2].

In this regard, our research group has focused on the development of a library of amphiphilic compounds derived from 4-hydroxyproline and proline mimetic amino-acids. Herein, their synthesis will be described and their permeation enhancement profile, using the model drug naproxen, will be presented [3]. Future efforts will be directed to the development of optimized structures, evaluation of their cytotoxicity profile and physico-chemical characterization.

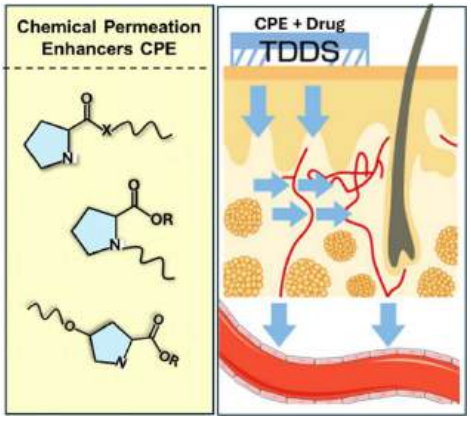

Fig. 3. Representation of TDD.

Acknowledgments: This work received financial support from PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through project UID/50006/2025 DOI 10.54499/UID/50006/2025 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos. Bárbara Sampaio thanks FCT for PhD grant 2024.04857.BD.

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MDR - D2 - F05
Synthesis of fluorinated partially saturated bicyclic drug scaffolds

Maryam Butt
Loughborough University, UK

Heterocyclic compounds containing nitrogen and fluorine are useful for the synthesis of many groups of drugs. In this research, the focus is on the synthesis of novel carboxamide derivatives of fluorine containing benzofused partially saturated heterocyclic rings **[1]**. The efficiency of fluorine containing molecules as pharmaceutical drugs is undeniable and every year new fluoro-pharmaceuticals drugs are introduced into the market after FDA approval **[2]**.
In this study, fluorine containing benzofused dihydropyrazine or dihydrothiazine rings will be synthesized. First, pentafluorobenzoyl chloride will be reacted with a range of substituted amines or anilines to form amides which was then reacted with either ethylene diamine or 2-aminoethanethiol to form benzofused rings by tandem S_NAr (Scheme 1). The potential for the aminoethylthio adduct to undergo Smiles rearrangement will be investigated. If ring does not occur, the intermediate pendant amine group will be reacted with a range of acylating agents to give an alternative series of scaffolds.
The synthesized compounds will then be studied not only for their mechanisms of formation but also for synthetic applications in drug discovery. Their inhibitory activity will be evaluated against the *Trypanosoma cruzi* parasite. *T. cruzi* is the causative agent of Chagas disease (CD), a potentially life-threatening and Neglected Tropical Disease. This disease is mostly affecting the population in South America where the disease is endemic.
The synthesized compounds will be evaluated through *Trypanosoma cruzi* lysyl-tRNA synthetase. This assay uses a pyrophosphatase enzyme to hydrolyse pyrophosphate. Accordingly, the free phosphate detected via a chemical reaction using Biomol Green. The synthesized compounds will be analysed by IR, MS, ^{1}H-, ^{19}F- and ^{13}C-NMR spectroscopy to determine their structures.
Fig 1: Mechanism of synthesis of Fluorinated Partially Saturated Bicyclic Drug Scaffol

Scheme 1:

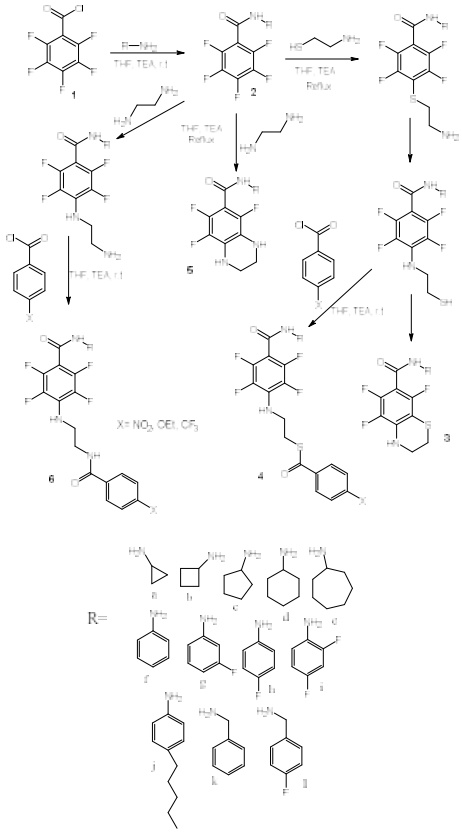

Fig 1: Mechanism of synthesis of Fluorinated Partially Saturated Bicyclic Drug Scaffolds

[1]Müller K., Faeh C., Diederich F. Fluorine in Pharmaceuticals:Looking Beyond Intuition. *Science.* **2007**, 317, 1881–1886.
[2]Inoue M, Sumii Y, Shibata N. Contribution of organofluorine compounds to pharmaceuticals. *ACS Omega*. **2020**, 5,10633–10640.

MDR - D3 - O01
Synthesis and application of large, water-soluble [$Fe^{II}_4L_6$] tetrahedra

Jack D. Wright[1], George F.S. Whitehead[1], Edward O. Pyzer-Knapp[2], Imogen A. Riddell[1]
[1]Dept. of Chemistry, The University of Manchester,UK; [2]Xyme, UK

Self-assembled metal-organic cages (MOCs) are excellent receptors for a wide variety of guests including ionic and polyaromatic molecules. The good guest selectivity and affinity reported in many cases has led to the proposed use of MOCs in medicinal and environmental remediation settings. The majority of the MOCs reported to date are, however, primarily soluble in organic solvents and exhibit poor aqueous solubility or stability thus making them incompatible with many biological and environmental applications. We have developed an extensible synthetic strategy that allows access to a family of Fe_4L_6 tetrahedra that exhibit high aqueous solubility and large, accessible hydrophobic cavities. These water-soluble MOCs support ongoing efforts in our group to develop clean supramolecular catalysts as well as pursue biological applications of MOCs.
Here, we focus on the encapsulation of established hydrophobic pollutants in a bid to develop a novel strategy for wastewater purification. These pollutants include tonalide a ubiquitous chemical employed in hygiene products and unmetabolized hormones from medicines. These chemicals are known to be poorly removed by current water treatment processes resulting in detrimental effects on the environment. We describe a data driven approach that allows design and synthesis of **MOC 1** (Fig 1),[1] a class-leading water-soluble MOC with an appropriately sized, hydrophobic cavity to accommodate our target guests. ITC analyses of guest binding within **MOC1** supports an enthalpically driven process consistent with a non-classical hydrophobic effect.
Building on initial results with **MOC 1** we go on to demonstrate the generality of our synthetic approach enabling a series of water-soluble cages to be synthesised and evaluate binding of a wider variety of guest molecules within this class of MOC.

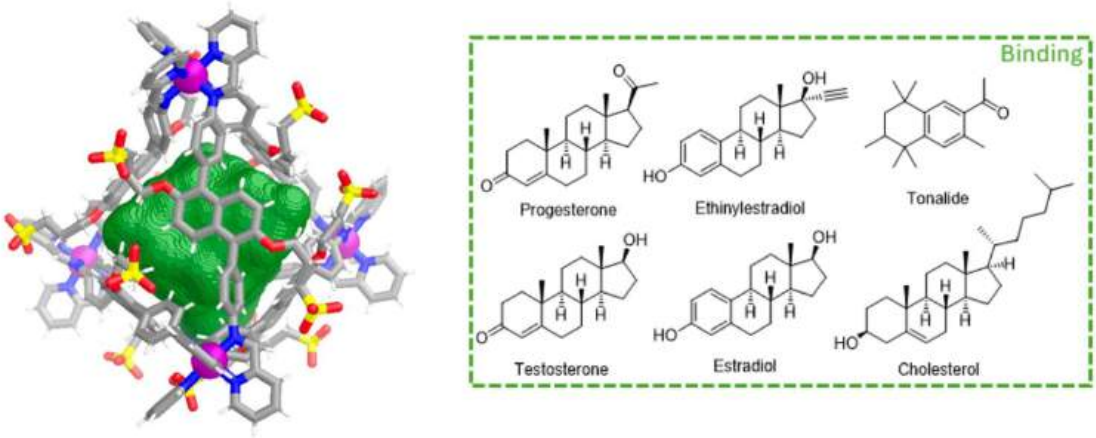

Fig. 1. Single crystal X-ray structure of **MOC 1** showing void cavity as shaded green mesh and a selection of guest molecules reported to bind within **MOC 1.**

[1]Wright, J.D.; Whitehead, G.F.S.; Pyzer-Knapp, E.O.; Riddell, I.A. *Cell Rep. Phys. Sci.* **2025***, 6,* 102404.

MDR - D3 - O02
Stabilising divalent carbodications through donor-coordination

Florian Mulks[1]
[1]*Institute of Organic Chemistry, RWTH Aachen University, Germany*

It has been more than a century since the discovery of carbocations (Gomberg), and we are working on a project to remove even more electrons from carbon. Divalent geminal carbodications can be handled using strongly electron-donating substituents (Loh, Bertrand) or by masking with donor ligands (Gleichmann, Petz, Neumüller, Frenking, Alcarazo, …), or a combination of these approaches (Maas, our lab). We use donor ligands to enable the scalable synthesis of masked *gem*-carbodications, thereby leveraging their exceptional reactivity. In a one-pot procedure, we synthesised diaminocarbodication (DAC^{2+}) nucleophile adduct ditriflates $DACNu(OTf)_2$ from simple urea derivatives on a 100 mmol (~50 g) scale. Our approach provides a convenient and efficient route to these potent Lewis acids. The inherent divalent carbodication character can be unleashed in substitution reactions. A pronounced chelation effect was observed in the 2,2'−bipyridyl adduct, marking a first trigonal bipyramidal carbon example. The pyridine unit in $DACPy^{2+}$ reacts with “softer” nucleophiles, while substitutions at the DAC^{2+} carbon occur with “harder” nucleophiles. It is challenging to provide a comprehensive description of such ambident reactivity, given the limited applicability of the HSAB principle in the field of organic chemistry. We have developed a new framework derived from Fukui functions to localise what we call electronic hardness and softness which helped better understand ambident organic reactivity. The high ion affinities of our compounds position them as competitive soft and hard acids. Highly efficient applications in amide couplings and Zincke reactions were demonstrated.

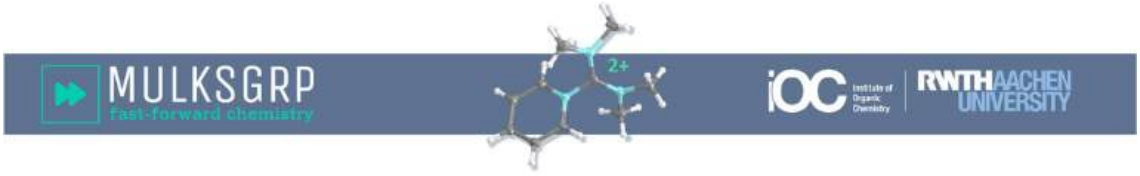

Fig. 1. Pyridine-stabilised diiminium salts were established as conveniently available and highly reactive examples of carbodications.

This work was supported by the “Fonds der Chemischen Industrie” through a Liebig Fellowship (Li 210/01) to F.F.M. and by the RWTH Aachen through HPC computing resources and an AROP fellowship.

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[4]Florian F. Mulks, *Chem* **2024**, *10*, 2724.

MDR - D3 - O03

Effect of aromatic substitution on spin crossover in [Fe(H_2Bpz_2)$_2$(bipy-R)] iron(II) complexes

Mengmeng Wang[1], Youssef Draoui[1], Koen Robeyns[1], Aurelian Rotaru[2], Dominik Maskowicz[3], Miroslaw Sawczak[3], Rafał Jendrzejewski[3], Yann Garcia[1]

[1]Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis (IMCN/MOST), Université catholique de Louvain, Belgium; [2]Dept. of Electrical Engineering and Computer Science and MANSiD Research Center, "Stefan cel Mare" University, Romania; [3]Photophysics Dept., The Szewalski Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Poland

Spin crossover (SCO) complexes are promising for applications in data storage, sensors, and molecular electronics due to their ability to reversibly switch spin state between high-spin (HS) and low-spin (LS) in response to changes in temperature, pressure, or light, accompanied by variations in electronic structure, magnetism, and color.[1] The spin transition behavior is mainly governed by ligand field strength and intermolecular cooperative interactions, necessitating systematic studies to understand the structure–SCO property relationship.[2] Aryl groups, characterized by their unique π-conjugation, steric effects, and fluorescence properties, play a crucial role in modulating the structure, electronic and photophysical properties of complexes. In this work, we introduce phenyl (phen), 1-naphthyl (1-nap), 2-naphthyl (2-nap), and anthryl (an) groups into the spin crossover (SCO) complex [Fe(H_2Bpz_2)$_2$(bipy)] (H_2Bpz_2 = dihydrobis(1-pyrazolyl)borate, bipy = 2,2′-bipyridine) in the C5 and C5' position of the bipy ligand connected by C=N imine bond to afford four Fe(II) complexes [Fe(H_2Bpz_2)$_2$(bipy-R)] (R = phen, **1**; R = 1-nap, **2**; R = 2-nap, **3**; R = an, **4**) and investigated their SCO properties (Figure 1). Magnetic measurements, ^{57}Fe Mössbauer, and Raman spectroscopy reveal that complexes **1** and **3** undergo one-step spin transition with ~57%/50% completeness and $T_{1/2}$ = 139 K/152 K. Complexes **2** and **4** exhibit two-steps gradual SCO with ~45%/30% completeness ($T_{1/2}$ = 242 K/289 K) for the first step and ~29%/50% completeness ($T_{1/2}$ = 137 K/176 K) for the second step. Unique crystal stacking patterns, different π⋯ π interactions, and electron effect raised by aromatic substituents and their influence on SCO behavior in the series complexes were discussed.

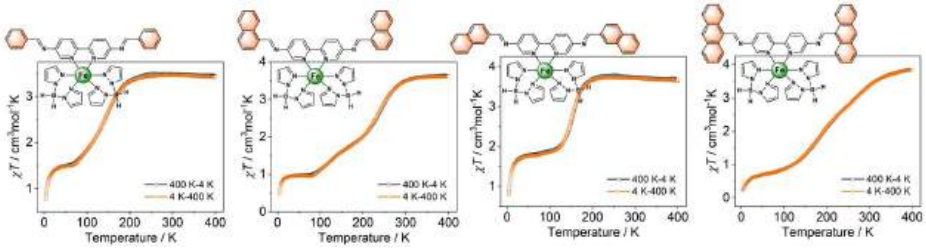

Fig. 1. The complexes referred to in this work and their $\chi_M T$ *vs*. *T* plots.

[1]Li, W.; Li, X.; Wang, M.; Bi, Y.; Garcia, Y. *CrystEngComm,* **2025**,*27*, 6848–6864.
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MDR - D3 - O04
Functionality fine-tuning in 1,2,3-triazolate-based coordination frameworks

Richard Röß-Ohlenroth[1], Dirk Volkmer[1]
[1]University of Augsburg, Germany

The 1,2,3-triazolate linker forms a whole range of different metal-organic frameworks (MOFs) with isotypic $M(ta)_2$-type structures.[1] Incorporation of metal ions such as Mg, Cr, Mn, Fe, Co, Ni, Cu, Zn, and Cd results in frameworks with subtle variations in pore sizes and apertures, rendering them attractive for gas separation, storage, and sensing applications. In addition, these MOFs feature a wide range of fascinating physical properties, i.e. electric conductivity,[2] spin-crossover transitions,[3] ferromagnetism,[4] and Jahn-Teller distortions.[5] Herein, we highlight the diverse functionalities of these frameworks and discuss recent strategies that enable their fine-tuning and manipulation. For instance, the introduction of 1,2,3-triazolate linker molecules with increased steric demand enables a controlled modulation of the spin-crossover behaviour,[6] as well as the Jahn-Teller distortions in $Fe(xta)_2$- (Figure 1a) and $Cu(xta)_2$-type structures, respectively.[7] Moreover, $Mn(ta)_2$, already intensively investigated for magnetic frustration and spin liquid properties (owing to its centered pyrochlore lattice),[8] was recently shown to efficiently separate H_2/D_2 gas mixtures via quantum sieving (Figure 1b).[9]

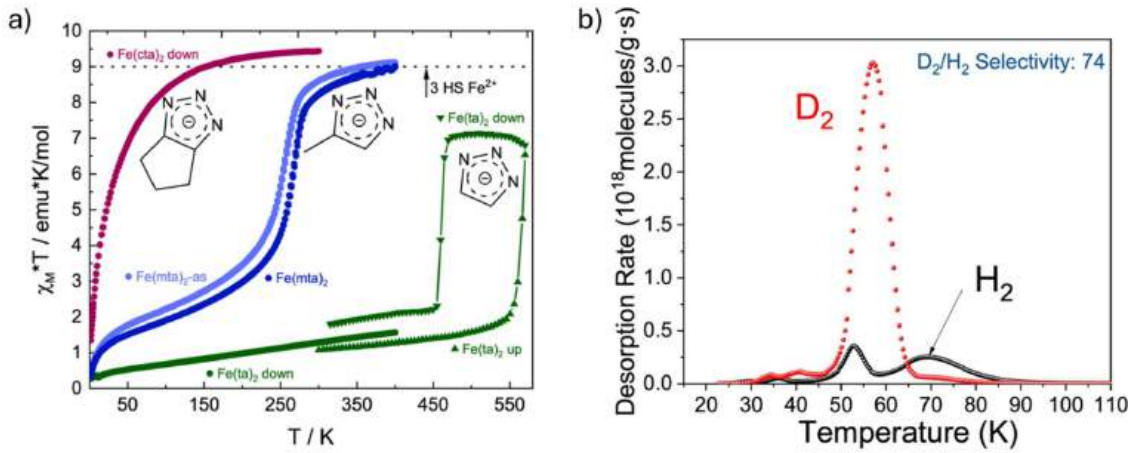

Fig. 2. Magnetization curves showing the effect of different steric demands of functionalized triazolate ligands on the spin-crossover transition of $Fe(xta)_2$-type frameworks (a). Enrichment of a 5:95 ratio H_2/D_2 mixture to 75% D_2 in a single cycle with $Mn(ta)_2$ (b).

[1]O. M. Yaghi et al. *Chem. Eur. J.* **2012**, *18*, 10595.
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[4]J. R. Long et al. *Nat. Chem.* **2021**, *13*, 594.
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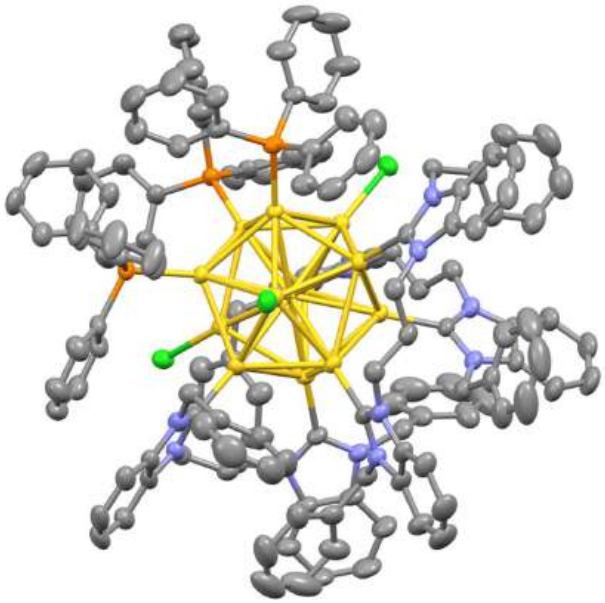
MDR - D3 - O05
Enhancing diversity in organometallic, atomically precise gold clusters

Giulia Saggiotti[1], Matteo Bevilacqua[2], Andrea Biffis[3]
[1]*Dipartimento di Scienze Chimiche, Università di Padova, Italy*

Atomically precise gold nanoclusters (Au NCs) are a class of well defined molecules featuring a core of gold atoms stabilized by a ligand shell. These molecules exhibit high chemical and electrochemical stability, photoluminescence and chirality, which can be potentially exploited in numerous applications. These properties are generally related to the use of different types of ligands, which from the more common thiolates and phosphines have been recently extended to carbon-based ligands, such as alkynyls or N-heterocyclic carbenes (NHCs). However, access to new organometallic clusters of this kind is still restricted by the limited availability of reliable, high-yielding synthetic methodologies.
To overcome this hurdle, we have embarked in a systematic study of the reactivity of well known and preformed Au NCs with carbon-based ligands/ligand precursors displaying different electronic and steric features. This strategy has proved useful to enable access to peculiar Au NCs which cannot be formed otherwise via direct methods. Indeed, we have recently succeeded in synthesizing mixed PPh_3 and NHC ligated Au NCs through a reaction sequence which allows to control both composition and nuclearity.[1] We have also disclosed the preparation of the first NHC-stabilized Au NC bearing gold-methyl bonds.[2] In this contribution, highlights will be provided on the electrochemical,[3] optical and medicinal properties of these Au NCs, as well as on the effect of tailored ligand substitutions in the cluster shell.



To further expand the field of organometallic AuNCs, we are also investigating the synthesis of unprecedented clusters stabilized by alternative neutral carbon-based ligands, such as isonitriles. Preliminary results in this direction will be reported as well.

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[3]Reato, M. et al. *Electrochimica Acta* **2025**, DOI 10.1016/j.electacta.2025.147562.

MDR - D3 - O06
Empowering cheap transition metals for catalysis by tuneable coordination in zeolites

Max Bols[1], Alexander Heyer[2], Dieter Plessers[3], Bert Sels[3], Kristine Pierloot[3], Edward Solomon[2]
[1]Ghent University, Belgium; [2]Stanford University, USA; [3]KU Leuven, Belgium

Copper and iron are highly accessible in the Earth's crust, but they are far removed from the 'Goldilocks' zone for heterogeneous catalysis occupied by the likes of platinum, palladium, iridium, rhodium, etc. This does not, however, disqualify iron and copper from performing spectacular catalysis, provided they are well surrounded.[1] This presentation will show how single copper and iron sites in zeolites look and behave very differently under the influence of their coordination to zeolite exchange sites.
Both copper and iron embedded in zeolites activate small molecules like N_2O, O_2 and CH_4, and the zeolite matters. Iron forms ferryl oxo sites from N_2O that do an H-abstraction from methane at room temperature.[2] While the active site looks simple, its electronic structure and thus reactivity is highly sensitive to the geometry of the exchange site in which it is embedded.[2,3,4,5] This electronic structure was investigated by numerous spectroscopies (Mössbauer, VTVH-MCD, NRVS, XAS, UV-Vis, ...) leading to molecular level insight and models that are uniquely experimentally calibrated.[1,2,3,4,5] Interesting effects are derived including driving force contributions to intrinsic barriers and entatic state effects.[2,3,4,5]
Copper sites are more challenging to study on the same fundamental level, since a larger variety of sites forms and these are more dynamic. Consequently, consensus in literature is further out of reach. Some of the debated aspects on O_2 and H_2O activation, and on the pathway for H-atom abstraction will be presented.[6,7] Interesting correlations relating geometric structure to electronic structure (incl. spin state)[8], and then to reactivity, will be critically evaluated.

This work was supported by the Flemish Science Foundation (FWO) and the National Science Foundation (NSF).

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[2]Snyder, B. et. al *Nature* **2016**, *536*, 317–321.
[3]Bols, M. et. al *J. Am. Chem. Soc*. **2018**, *140*, 38, 12021–12032.
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[5]Bols, M. et. al *Nature Catal.* **2021**, *4*, 332–340.
[6]Heyer, A. et. al *J. Am. Chem. Soc*. **2024**, *146*, 31, 21208–21213.
[7]Phung, Q. et. al; *J. Am. Chem. Soc*. **2025**, *15*, 2, 1249–1264.
[8]Heyer, A. et. al *J. Am. Chem. Soc*. **2024**, *146*, 9, 6061–6071.

MDR - D3 - O07
Magnetic dendrimers: Tacking the challenge of synthesis and characterization

Valérie Marvaud[1], Cédric Pécou[1], Ingrid Suzana[1], Moritz Malischewski[2]
[1]Parisien de Chimie Moléculaire, Sorbonne Université, Paris, France; [2]Fachbereich Chemie, Freie Universität, Berlin, Germany

Despite the vast potential of dendrimer chemistry, magnetic dendrimers remain relatively scarce in the literature due to perplexing challenges in their synthesis and characterization. Consequently, designing such multimetallic and monodisperse starburst architectures endowed with magnetic properties poses a significant challenge. Initial efforts focused on the coupling of tetra- and penta-nuclear complexes, with promising results. The Gd5Cu16 complex showed magnetization compatible with S = 51/2, while the Tb5Cu16 equivalent showed single molecule magnetic behavior but no crystallographic structure.
Using a supramolecular "complex as ligand" approach, we successfully address the challenge through synthesis, characterization (including X-ray diffraction) and investigation of magnetic dendrimers. Our synthetic strategy relies predominantly on oxalate-based coordination chemistry as the core of the architecture, alongside trinuclear complexes, LnCo2, for the branches, which exhibit single-molecule magnetic properties. The integration of these building blocks allows the formation of supramolecular and dendritic assemblies. The versatility of this approach allows the anticipation of properties based on the choice of metal cations involved in the structure, such as single molecule magnets or giant spin values. Consequently, we have obtained hetero-tri-metallic dendrimers, MLn3Co6 and ZrLn4Co8 (where M=Co or Cr, and Ln=La, Tb, Dy, etc.), fully characterized by X-ray diffraction. The observed magnetic properties are in good agreement with theoretical models, suggesting potential applications in information storage, quantum computing or magnetic refrigeration.

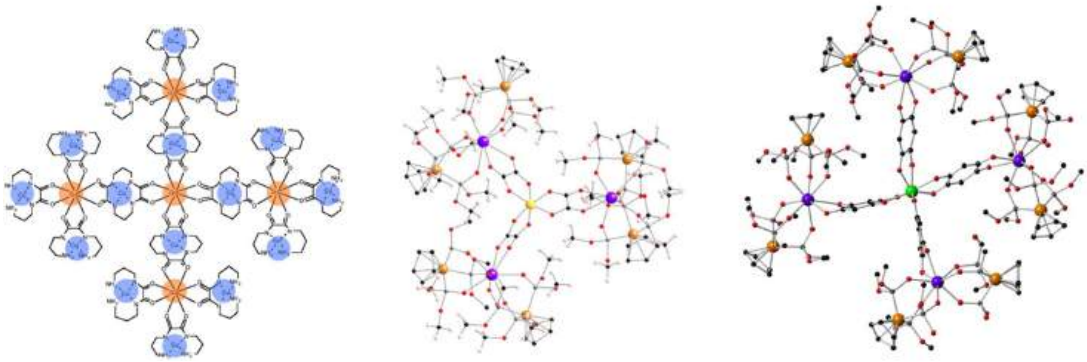

Fig. 1. Magnetic dendrimers Gd5Cu16, CrGd3Co6 and ZrLn4Co8 (X-Ray structures)

This work was supported by the Centre National de la Recherche Scientifique (CNRS), Sorbonne Université in Paris, Freie Universität in Berlin, and the Agence Nationale de la Recherche (ANR) under the grants [SMAC and MagDen]. We gratefully acknowledge their financial support.

[1]I. Suzana, C. Pécou, M. Malischewski, V. Marvaud et al. , *Inorg. Chem. Front.* DOI : https://doi.org/10.1039/D5QI02242H
[2]D. Astruc, E. Boisselier, C. Ornelas, *Chem. Rev.* 2010, *110*, 1857 and ref. therein.

MDR - D3 - O08
Reactivity studies of a main-group lead hydride and a bimetallic di-iron dihydride complex

Hsueh-Ju Liu[1]
[1]*Dept. of Applied Chemistry, National Yang Ming Chiao Tung University, Taiwan*

Herein, we present our recent studies on the reactivity of two distinct classes of metal hydrides developed in our laboratory, highlighting how ligand design enables unusual electronic structures and reactivity patterns.
First, we describe a dianionic pincer-type {NNN} ligand-supported Pb(II) platform that enforces an open coordination site along the z-axis. This structural feature is closely related to our previous work on ligand-unsupported extended metal atom chains (EMACs),[1] in which metal–metal chain growth occurs perpendicular to the ligand plane. The resulting neutral Pb(II) synthon serves as a versatile precursor to a range of Pb(II) complexes, including a rare and highly reactive Pb(II) hydride (Fig. a).[2] Notably, this lead hydride displays pronounced nucleophilicity and is capable of cleaving strong carbon–halogen bonds, including C–F bonds. We demonstrate controllable hydrodefluorination of both C(sp2)–F and C(sp3)–F bonds under distinct reaction conditions, providing mechanistic insight into main-group hydride-mediated C–F bond activation.
Second, we introduce a low-coordinate di-iron dihydride complex (Fig. b) stabilized by a tethered bis-cyclopentadienyl ligand framework, which is synthesized via a recently reported di-iron trihydride precursor.[3] This bimetallic hydride system exhibits pronounced metal–metal cooperativity toward small-molecule activation, enabling transformations relevant to the development of synthetically useful catalytic processes. Together, these studies illustrate how tailored ligand environments can unlock unconventional hydride reactivity across both main-group and transition-metal platforms.

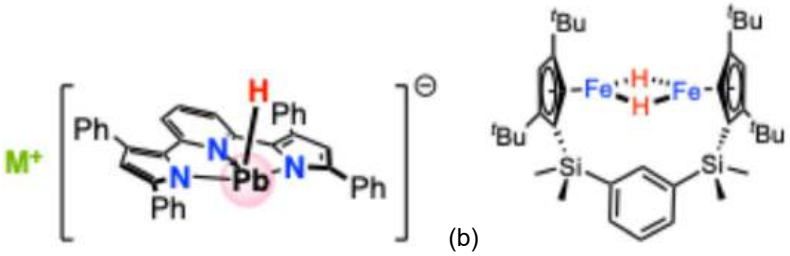

Fig.1. Structures of (a) the anionic lead hydride and (b) an Fe_2H_2 complex.

[1]Chang, W.-C.; Raj. A.; Hiramatsu, H.; Li, H.-J.; Ziegler, M. S.; Lin, Y.-C.; Huang, S.-C.; Liu, H.-J. *Chem. Commun.*, **2020**, *56*, 6786–6789.
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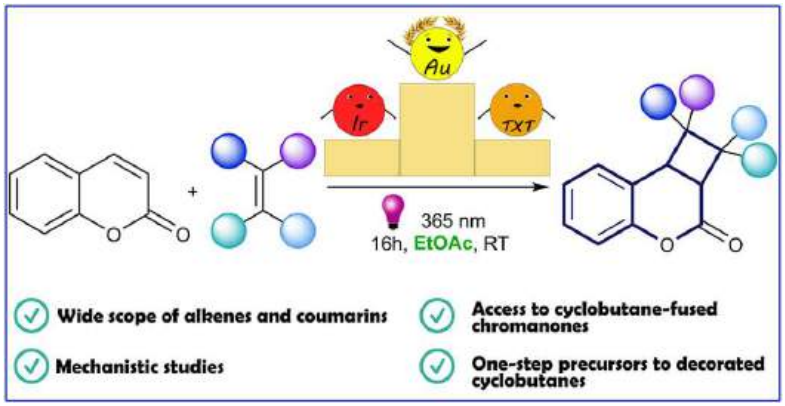
MDR - D3 - O09
The [M(NHC)Cbz)] architecture (M= Au and Cu; Cbz = carbazolyl): Advances in EnT photocatalysis

Tommaso Ruggiero[1], Vladislav Voloshkin[1], Ekaterina Martynova[1], Yuan Zhao[1], Nikolaos Tzouras[1], Steven P. Nolan* [1]
[1]*Dept. of Chemistry and Center for Sustainable Chemistry, Ghent University, Belgium*

Energy transfer photocatalysis has emerged as a powerful platform for a wide variety of transformations. Catalysis enabling such transformations are based on Iridium centers and these constitute the state-of-the-art. We have uncovered that simple architectures revolving around Group 10 can enable such triplet energy transfer processes. The inner working of these systems , how they can be simply synthesised and to what extent they act as mimics of their Ir conterparts will be discussed.



MDR - D3 - O10
Design of isoindole-based *N*-heterocyclic ligands for bioactive bimetallic complexes

Mélaine Wang[1,2], Jalloul Bouajila[3], Agathe Figarol[4], Isabelle Jourdain[2], Michael Knorr[2], Mohamed Othman[1]
[1]URCOM, France; [2]Institut UTINAM, France; [3]Laboratoire de Génie Chimique, France; [4]Femto-ST, France

The discovery of cisplatin has stimulated intensive research on metal-based therapeutics, aiming at the development of more efficient and less toxic metallodrugs.[1] One promising strategy consists in combining biologically active organic scaffolds with transition metal fragments to generate synergistic metal-ligand systems. In this context, isoindole derivatives represent attractive *N*-heterocyclic frameworks with significant pharmaceutical potential.[2]
In this work, we report the synthesis, structural characterization, and biological evaluation of homobimetallic Co-Co, Pt-Pt complexes, as well as heterobimetallic Fe-Pt complexes and Pt(0) π-complexes incorporating an isoindole unit, synthesized from alkyne-functionalized isoindole ligands. The new compounds were fully characterized by IR, multinuclear NMR spectroscopy, and single-crystal X-ray diffraction.[3] The structural features of these complexes reveal diverse metal-metal interactions and coordination modes, offering valuable insights into structure-activity relationships.
The cytotoxic properties of the complexes were evaluated against three human cancer cell lines (HCT116, WM266-4, and LS174T) and their toxicity toward healthy cells was also assessed in order to evaluate their selectivity.[4] These results highlight the potential of isoindole-based bimetallic complexes as promising platforms for the development of novel metallodrugs.

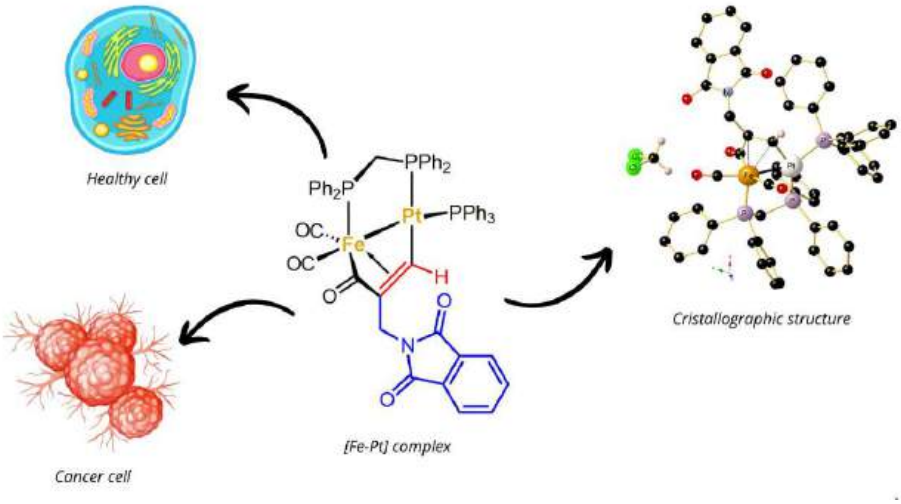


Fig. 1. A selective [Fe-Pt] complex - structure and cancer cell targeting

This work is supported by Region Normandie and EPE Bourgogne-Franche-Comté. The authors also thank Prof. Carsten Strohmann's group at TU Dortmund University for single-crystal X-ray diffraction analyses.

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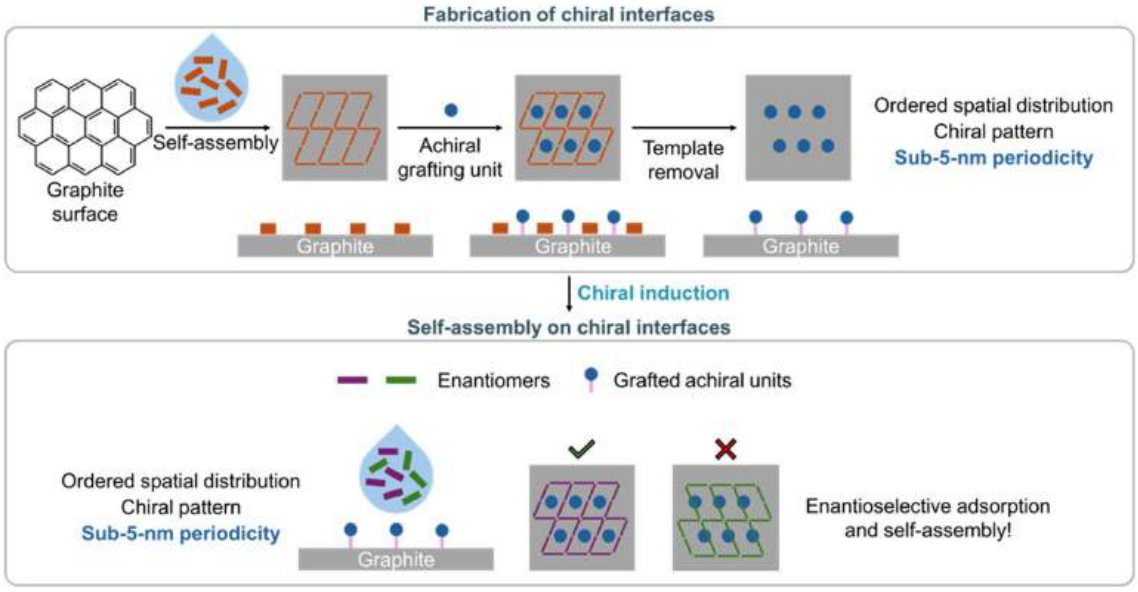
MDR - D3 - O11
Enantioselective interactions on chiral nanopatterned surfaces

Kobe Peeters[1], Kunal S. Mali[1], Kazakuni Tahara[2], Steven De Feyter[1]
[1]Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Belgium; [2]Dept. of Applied Chemistry, School of Science and Technology, Meiji University, Japan

Homochiral surfaces serve as crucial platforms not only for enantiomeric separations and asymmetric heterogeneous catalysis but also as experimental grounds for investigating the expression, transmission, and amplification of chirality on solid surfaces from the bottom up. While covalent bond-based chiral modification of solid substrates offers high stability, it remains relatively underexplored, particularly from a nanoscale patterning standpoint. This underscores the necessity for developing systematic approaches for chiral covalent surface modification and conducting comprehensive nanoscale characterization. Surfaces patterned with chiral features at sub-5-nanometer periodicities hold considerable potential in chiral separations, sensing, and catalysis. Moreover, exploring the adsorption and self-assembly of organic molecules on such patterned surfaces will yield valuable insights into the mechanisms of chiral transmission from the surface to surface-bound entities, a critical aspect in understanding enantioselective adsorption. The project aims to develop systematic methodologies for creating patterned surfaces with precise control over the arrangement of chiral functional groups and to use these surfaces for conducting proof-of-concept experiments on enantioselective self-assembly.



Acknowledgements: Financial support from the Research Foundation – Flanders (FWO) through a PhD grant (14960654) and project G0A5I24N is gratefully acknowledged.

MDR - D3 - O12
Chiral metal-organic frameworks (MOFs) enhance oxygen evolution reaction through CISS effect

Alessio Nicolini[1], Martina Campi[1,2], Valeria Iacomini[1,2], Roberto Biagi[2], Marco Borsari[1], Andrea Cornia[1], Simone D'Agostino[3], Lara Gigli[4], A. Gupta[5], R. Naaman[5], Adele Mucci[1], Paolo Zardi[1], F. Tassinari[1]
[1]Dept. of Chemical and Geological Sciences & INSTM RU, UniMORE, Modena, Italy; [2]Dept. of Physics, Informatics and Mathematics, UniMORE, Modena, Italy; [3]Dept. of Chemistry G. Ciamician, UniBO, Bologna, Italy; [4]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Italy; [5]Dept. of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel

Spin-polarized currents can have an important impact on the efficiency of spin-dependent catalytic processes. For example, during Electrochemical Water Splitting (EWS) they favour the formation of O_2 in its triplet ground state (S=1) and lower the activation energy for the Oxygen Evolution Reaction (OER).[1] However, the main shortcoming of the studies conducted so far is the lack of well-defined structural data. To overcome this problem, we exploited the spin-polarized currents produced by chiral Metal-Organic Frameworks (MOFs) which act as spin-filters thanks to the Chiral Induced Spin Selectivity (CISS) effect.[2] As further advantages, MOFs can possess high surface areas and can be based on cheap and abundant first-row transition metals, a key factor to substitute state-of-the-art catalysts containing Pt or Ir. In this work, we isolated a chirally functionalized nickel(II)-based 3D MOF (Ni-C) and its achiral analogue (Ni-A) using dicarboxylic organic linkers carrying chiral and achiral side chains, respectively (H_2C and H_2A in Fig. 1). Although Ni-C and Ni-A possess the same structure, Ni-C exhibits a higher catalytic activity. Notably, mc-AFM measurements showed that Ni-C is a CISS-active spin-filter catalyst for OER, with spin-polarization of ~50%. This important result paved the way for further studies aiming at designing new chiral MOFs with improved catalytic activity. For example, we pursued a more efficient transfer of chirality to the metal centres using an axially chiral ligand (H_2L in Fig.1). Additionally, we designed and isolated the new dipyrazolate ligands in Fig.1, and employed them as linkers to assemble cobalt(II)-based MOFs with increased stability and conductivity with respect to dicarboxylate MOFs. In this contribution we will show the most interesting results we obtained in the last year.

Funding: Funded by PNRR–M4C2INV1.5, NextGenerationEU-Avviso 3277/2021 -ECS_00000033-ECOSISTER-spk2.

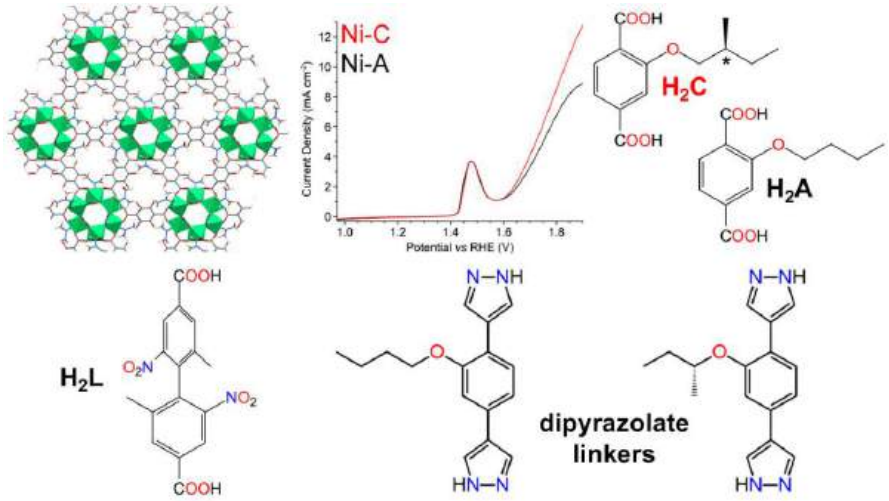


Fig. 1. Structure of the Ni-based MOFs and of the organic linkers, and catalytic activity of Ni-C and Ni-A.

[1]Vadakkayil, A. *et al.*, *Nat. Commun.* **2023**, *14*, 1067.
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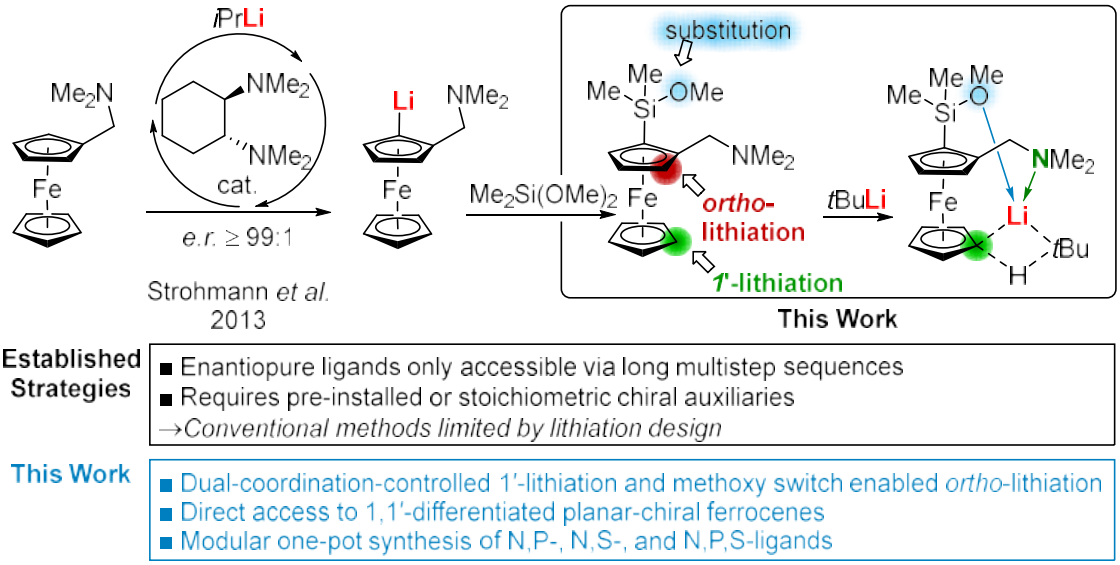
MDR - D3 - O13

Selective 1'-lithiation of planar-chiral ferrocenes enabled by switchable coordination: The effect of a methoxy-silyl group

Paul Erik Schneider[1], Helene Gillner[1], Christopher Golz[2], Carsten Strohmann[1]
[1]Faculty of Chemistry and Chemical Biology, TU Dortmund University, Germany; *[2]Institute of Organic and Biomolecular Chemistry, Georg-August-Universität Göttingen, Germany*

Herein, we report that switching from a coordinating methoxy-silyl- to a non-coordinating trimethyl-silyl-group enables selective sequential 1′- and *ortho*-lithiation of planar-chiral ferrocenes. Planar-chiral ferrocenes are privileged scaffolds in asymmetric catalysis, yet access to modular, 1,1′-differentiated enantiopure derivatives remains limited.[1] While several positions on ferrocenes can nowadays be functionalized by transition-metal-catalyzed C–H activation,[2] 1'-substitution still exclusively relies on lithium chemistry. Existing routes depend on multi-step sequences, often involving auxiliary-controlled lithiations, which restrict substitution diversity and efficiency.[3] We present a coordination-controlled lithiation sequence exploiting the dual reactivity of a dimethylmethoxysilyl-substituted (aminomethyl)ferrocene. Depending on the lithium alkyl reagent, either selective 1′-deprotonation (*t*BuLi) or methoxy substitution occurs (MeLi), thus flipping a reactivity switch that enables a subsequent second *ortho*-lithiation (*i*PrLi). Combined NMR spectroscopy, X-ray crystallography, and DFT studies reveal cooperative amino/methoxy coordination as the origin of the observed 1'-regioselectivity. This mechanistically guided, one-pot protocol provides the first concise route to planar-chiral 1,1′-unsymmetrical ferrocenes, including N,P-, N,S-, N,O,S- and N,P,S-functionalized derivatives. It establishes a general reactivity-control concept, highlighting the potential of the present mechanism to guide future 1'-position-selective transformations. The enantiomerically pure access is backed up by an enantioselective lithiation of *N,N*-dimethyl(aminomethyl)ferrocene using catalytic amounts of the chiral diamine ligand (*R,R*)-TMCDA, affording planar-chiral ferrocenes with excellent enantioselectivity (*e.r.* ≥ 99:1).[4] An enantiomerically pure starting point is particularly advantageous, as the rigid ferrocene scaffold preserves the configurationally stable planar chirality throughout all downstream transformations.



Scheme 1. Strategy for accessing 1,1′-unsymmetrically substituted planar-chiral ferrocenes.

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MDR - D3 - O14

Excited-state dynamics of Iridium(III) photosensitizers bearing pH sensitive strong electron donating bipyridine ligand functionalized with n-heterocyclic imine and olefin

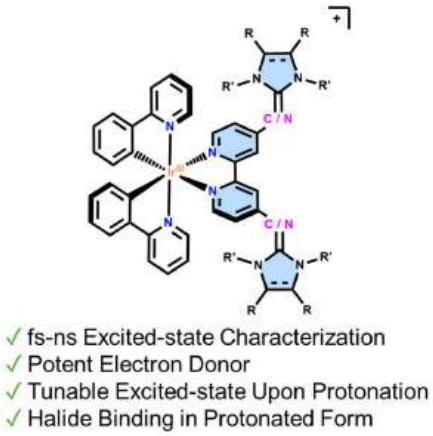
Sven Lempereur[1,2], Felix Glaser[1], Jonas H. Franzen[2], Leon Schondorf[2], Michael Siedl[2], Fabian Dielmann[2], Ludovic Troian-Gautier[1,3]

[1]Institut de la Matiere Condensee et des Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis (MOST), Universite catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium; [2]Institute of General, Inorganic and Theoretical Chemistry, Universitat Innsbruck, Innsbruck, Austria; [3]Wel Research Institute, Wavre, Belgium

Iridium(III) polypyridyl complexes are central to contemporary photoredox catalysis and optoelectronics, where precise control over excited-state energetics and charge-transfer character is essential. While extensive efforts have focused on electron-withdrawing ligand frameworks to enhance excited-state oxidizing power, the complementary use of strongly electron-donating diimine ligands remains comparatively underdeveloped, despite their potential to unlock new excited-state reduction pathways and electronic manifolds.[1,2] Addressing this imbalance requires ligand platforms that exert a pronounced electron-donating influence while remaining responsive to external stimuli.

Here, we investigate a new class of heteroleptic Ir(III) complexes incorporating highly electron-rich bipyridine ligands functionalized with either N-heterocyclic imine[3] (bpy-NHI) or N-heterocyclic olefin (bpy-NHO) substituents. A combination of spectroelectrochemistry, steady-state absorption and emission spectroscopy, and time-resolved spectroscopic techniques reveals that these substituents dramatically reshape both ground- and excited-state electronic structures. For $[Ir(ppy)_2(bpy\text{-}NHI)]^+$, the strong electron donor character suppresses the conventional bipyridine-centered reduction and leads to an unusual excited state predominantly localized on the cyclometalated ligands. In contrast, the bpy-NHO analogue exhibits a fundamentally different excited-state landscape, with charge transfer centered on the diimine ligand. The near-planar NHO–bipyridine framework gives rise to an intraligand charge-transfer (ILCT) absorption band, enabling excitation-wavelength-dependent excited-state behavior.

Importantly, protonation of the imine or olefin units effectively attenuates their donor strength, restoring photophysical properties resembling those of the parent $[Ir(ppy)_2(bpy)]^+$ complex. These protonation events, along with evidence for anion preassociation, are directly observable spectroscopically and demonstrate how second-sphere interactions can be leveraged to reversibly modulate excited-state character. Overall, this work establishes bpy-NHI and bpy-NHO ligands as powerful, stimuli-responsive platforms for engineering electronically diverse Ir(III) photosensitizers.



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MDR - D3 - O15
Luminescent complexes with imino/amino podands containing extended π systems

Augustin M. Mădălan
Faculty of Chemistry, University of Bucharest, Romania

Polydentate imino and/or amino ligands play a significant role in the design of homo- and heteropolynuclear complexes containing 3d and/or 4f metal ions. The imino ligands derived from o-vanillin and various diamines are typically bicompartmental ligands, allowing the synthesis of heterobinuclear 3d-4f complexes [1]. In mononuclear complexes with the metal ion hosted into the inner N_2O_2 compartment, the larger vacant $O_2O'_2$ compartment can act as a receptor not only toward other metal ions, but also toward hydrogen bond donors, for example, the aqua ligand arising from other complexes, amino groups or ammonium cations [2].
Within the category of podands, the tripodal ligands are molecules projected to encapsulate more fully their guest. The presence of extended □ systems as pendant arms of the ligands can contribute to the luminescent properties of the complexes [3] and, also, to non-covalent interactions with different chemical species.
In Zn(II) mononuclear complexes with the tripodal ligand resulted from the condensation of tris(2-aminoethyl)amine with 9-anthracenecarboxaldehyde, these non-covalent interactions of the anthracene moieties with solvent molecules or halide anions coordinated to the metal ion induce conformational changes of the ligand (Figure 1).

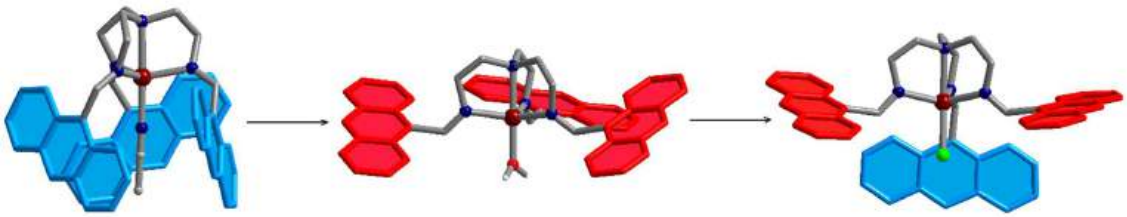

Fig. 1. Conformational changes of a tripodal ligand in Zn(II) mononuclear complexes induced by the solvent coordinated to the metal ion or by halogen-p interactions

Polydentate imino ligands possessing pendant arms with extended π systems can be used for the sequential synthesis of heteroleptic complexes taking the advantage of π–π interactions established by the pendant arms with the secondary ligand.

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MDR - D3 - O16

Thermo-/photo-responsive fluorescence and mechanical properties of dynamic organic crystals

Hsu-Chi Chang[1], Yu-Chun Chuang[1,2], Jye-Shane Yang[1,3]

[1]Dept. of Chemistry, National Taiwan University, Taiwan; [2]Scientific Research Division, National Synchrotron Radiation Research Center, Taiwan; [3]Center for Emerging Material and Advanced Devices, National Taiwan University, Taiwan

Dynamic organic crystals have emerged as a novel class of stimuli-responsive materials. However, mechanistic understanding of how molecules move under the constraints of a crystal lattice and noncovalent interactions to produce changes in structure and properties (e.g., shape, color, and conductivity) in response to external stimuli (e.g., light, heat, and pressure) remains limited, making rational molecular design challenging. A common obstacle is the loss of crystallinity after a phase transition.

We recently demonstrated that the rigid, H-shaped pentiptycene scaffold can enhance solid-state molecular mobility while preventing aggregation-caused quenching and maintaining good crystallinity. This makes pentiptycene-based molecular crystals useful for elucidating structure–property relationships. One example is a family of anthracene-pentiptycene hybrid systems (Figure 1),[1-4] which exhibit thermochromic or photochromic fluorescence as well as thermomechanical or photomechanical responses, including rotation, translation, bending, elongation, cracking, and jumping.

In this presentation, I will focus on the molecular motions involved in the polymorphic transition of one such system and the resulting fluorescence color changes and mechanical behavior. Specifically, the transition proceeds via a cooperative (maternsitic-like) mechanism involving molecular gear rotations between green- and yellow-emissive polymorphs. Depending on alkyl chain length, the relative energetics of the initial and the final states vary, leading to Hammond Postulate-like behavior. In addition, alkyl chain length influences crystal free volume and thus solvent inclusion. The structure–property relationships will be discussed.

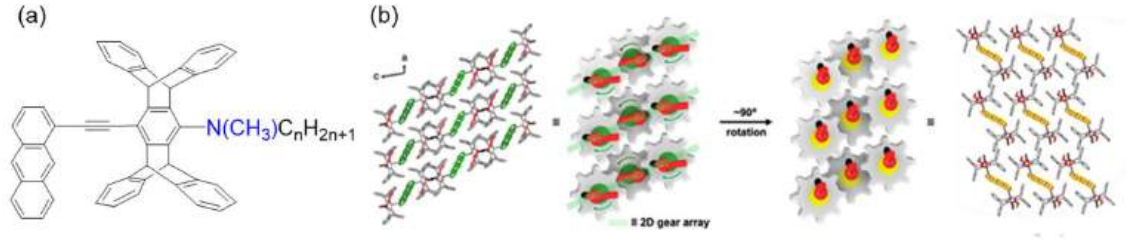

Fig. 1. (a) molecular structures of anthracene-pentiptycene hybrid systems; (b) molecular gear rotation drives a polymorphic transition from a green-emissive form to a yellow-emissive form.

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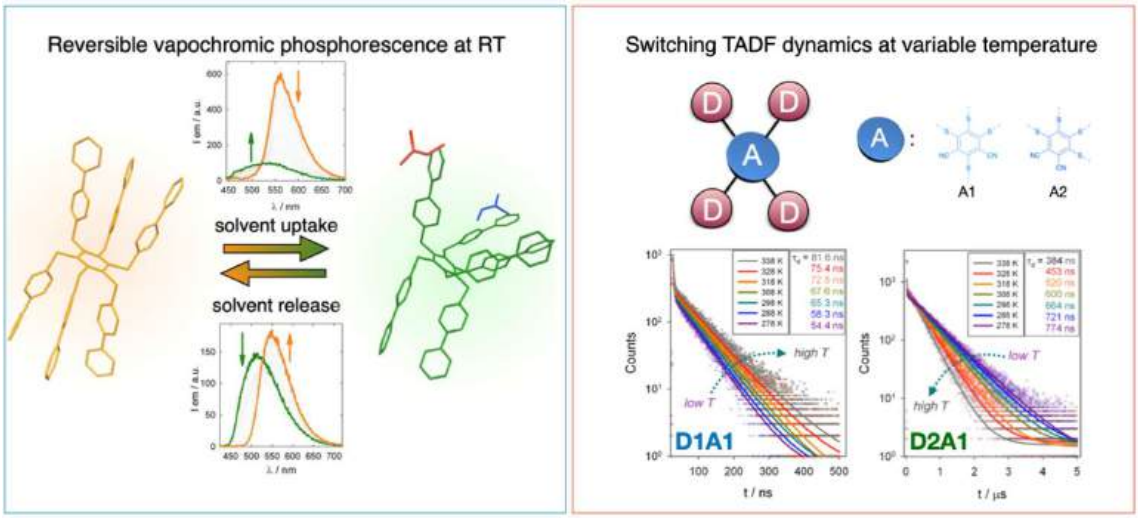
MDR - D3 - O17
Luminescent polysulfurated benzenes: A versatile platform for RTP and TADF materials

Andrea Fermi[1], Sultan Çetin[1], Giacomo Mastruzzi[1], Paola Ceroni[1], Simone d'Agostino[1], Fabrizia Negri[1], Sapna Gahlot[2], Marc Gingras[2]
[1]Dept. of Chemistry, University of Bologna, Italy; [2] Aix-Marseille Université, France

Polysulfurated benzenes represent a versatile, noble-metal-free scaffold for engineering high-performance triplet-emitting organic materials.[1-2]
In our recent research,[3] stimuli-responsive room-temperature phosphorescence (RTP) in the solid state is achieved by leveraging the structural flexibility achieved from a decorated persulfurated core. We show that the inclusion of solvent molecules triggers significant conformational changes, leading to a dramatic modulation of photophysical properties. Specifically, we report a distinctive vapochromic behavior at room temperature, driven by the reversible conversion between two intramolecular conformations. Experimental results and computational analysis suggest that the vapochromic response originates from a fundamental shift in the nature of the emitting triplet state.
In addition, the triplet excited state dynamics result dramatically affected by the introduction of electron donor-acceptor architectures, making polysulfurated compounds able to emit through thermally activated delayed fluorescence (TADF) not only in the solid state, but also in solution at RT.[4] Temperature-dependent time-resolved emission spectroscopy has confirmed that spin-forbidden processes depend crucially by the presence of peripheral substituents of different electronic nature, drastically affecting both intersystem crossing (ISC) and reverse intersystem crossing (rISC).
Our results establish polysulfurated benzenes as a scalable, all-organic platform for application in optoelectronic materials and highly sensitive solid-state sensing devices.



The national PRIN-PNRR "Enlightening" project (P2022PZ2MM) is acknowledged for funding.

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[4]S. Çetin, A. Zattarin, G. Mastruzzi, S. d'Agostino, P. Ceroni, A. Fermi, **2026**, *submitted*.

MDR - D3 - O18
FROG dyes: A new class of anionic near infrared fluorophores

Isaac Fuentes[1], Rui Tang[2], Megan S. Michie[2], Christina Lin[2], Mikhail Y. Berezin[2] and Vladimir B. Birman[1]
[1]Washington University, USA; [2]Washington University School of Medicine, USA

Fluorescence has become an indispensable tool in interrogating complex biochemical and biomedical phenomena through imaging-based studies. Fluorescence in the near-infrared (NIR) region (700 nm – 900 nm) is of great interest for its ability to image with higher sensitivity and an increased spatiotemporal resolution, which is oftentimes unobtainable through the ultraviolet and visible regions.[1,2] This optical window capitalizes on the low energy radiation of the NIR to achieve greater depth penetration, mitigate cellular damage, and reduce autofluorescence from biological tissues.
Historically, the NIR region has been dominated by the cyanine family following the success of FDA-approved Indocyanine Green; however, as science and technology advances there becomes a growing need for a more robust suite of available fluorophore scaffolds.[3,4] We have generated a new class of biologically relevant polymethine dyes that feature anionic 1,6-diheterophenalene-2,5-dione end groups.[5] The synthesis, spectroscopic data, and biological application of these dyes will be the focus of this presentation.

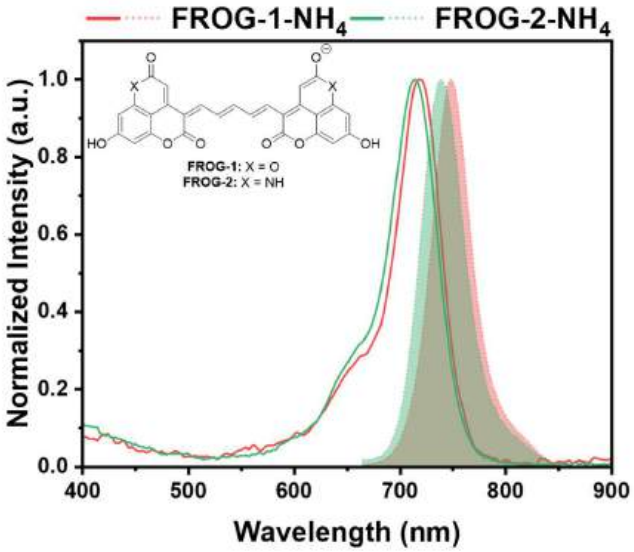

Fig. 1. Absorption (solid) and emission (dashed) profiles of FROG dyes in DMSO.

[1]Dai, M. *et al. Chem. Soc. Rev.* **2023**, *52*, 6344–6358.
[2]Xu, W. *et al. Angew. Chem. Int. Ed.* **2016**, *55*, 13658–13699.
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MDR - D3 - O19

Electrochemiluminescence of a unimolecular ruthenium(II)–labelled cucurbit[7]uril: From mechanistic insights to applications

Maria Vittoria Balli[1], Patrick Gruhs[2], Madhurima Jana[1], Chiara Capolungo[1], Pierre Picchetti[2], Papri Chakraborty[2], Emily Janz[2], Marco Neumaier[2], Manfred Kappes[2], Giovanni Valenti[1], Luca Prodi[1,3], Frank Biedermann[2]

[1]University of Bologna, Italy; [2]Karlsruhe Institute of Technology, Germany; [3]IRCCS Azienda Ospedaliero-Universitaria di Bologna, Italy

Electrochemiluminescence (ECL) has evolved from fundamental mechanistic studies into a central transduction technology for ultrasensitive bioassays,[1] yet diffusion-controlled encounters between luminophores and coreactants intrinsically limit ECL efficiency and, consequently, related biosensors' performance. Herein, we report a host–guest-based ECL-active construct, in which a tris(2,2′-bipyridyl)ruthenium(II) moiety is covalently tethered to cucurbit[7]uril *via* a flexible tetraethylene glycol linker,[2] yielding the unimolecular CB7–Rubpy. This design enables modulation of $[Ru(bpy)_3]^{2+}$ photophysical properties through its dynamic binding at the CB7 portal in the presence or absence of CB7-binding guests. Remarkably, ECL measurements with tri-*n*-propylamine as coreactant display a 163% signal enhancement compared to $[Ru(bpy)_3]^{2+}$ alone. Mechanistic studies attribute this enhancement to confinement of the coreactant within the CB7 cavity, promoting efficient homogeneous electron transfer, thereby overcoming diffusion-controlled limitations through spatial colocalization of luminophore and coreactant. These results are further translated into analyte-dependent modulation of ECL intensity upon competitive binding of small biomolecules, *e.g.*, nandrolone and spermidine, achieving detection limits down to 76 nM in aqueous media. This work establishes CB7–Rubpy as the first self-contained, recognition-responsive ECL emitter, introducing a supramolecular strategy for enhancing ECL efficiency while enabling highly sensitive, antibody-free detection of small biomolecules directly in solution, without any electrode surface modification.

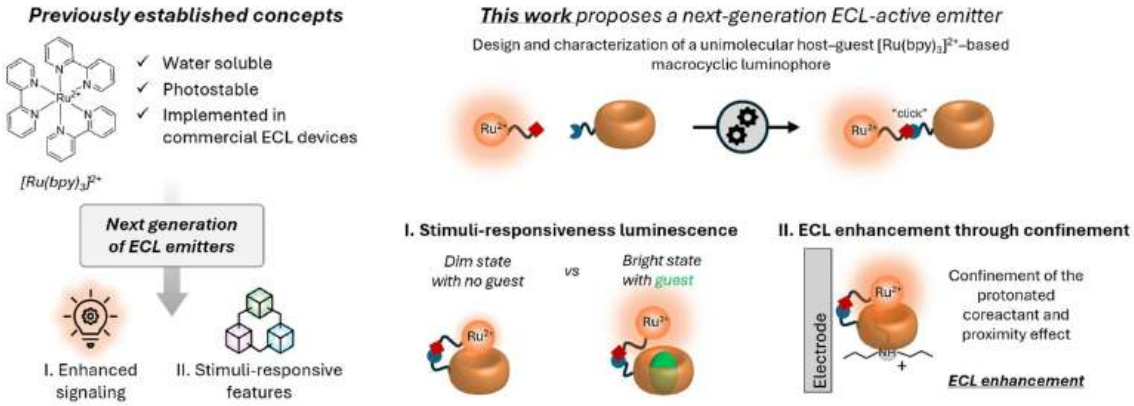

Fig. 1. Comparison between $[Ru(bpy)_3]^{2+}$ applications and the herein presented CB7–Rubpy tuneable luminescence and enhanced ECL output.

Acknowledgements: the European Union's Horizon Europe EIC Pathfinder Open program "ECLIPSE" (Grant Agreement No. 101046787) is acknowledged for financial support.

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MDR - D3 - F01
Needs determine the way: The Place of SF_4 in modern synthetic chemistry

Dmytro Volochnyuk[1,2,3,4], Serhiy Trofymchuk[1,2], Serhiy Ryabukhin[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Institute of Organic Chemistry, NAS of Ukraine; [3]Enamine Scientific Research Institute, Ukraine; [4]Taras Shevchenko National University of Kyiv, Ukraine

Sulfur tetrafluoride (SF_4) remains one of the most controversial fluorinating reagents. It is an extremely toxic, colorless gas that easily hydrolyzes to highly corrosive HF. Despite all those, SF_4 continues to see increasing industrial production and use (~2,000 tons annually, agrochemistry – 50%, pharm industry – 21%, others – 29% (10% liquid crystals)).
The practical and safety limitations of SF_4 drove the development of "safer" derivatives, including DAST, Morph-DAST, and XtalFluor-type reagents – many produced from SF_4 itself. However, replacing SF_4 with these analogues is not always a simple upgrade. In several high-value transformations, SF_4 remains uniquely effective, particularly for (a) carbonyl oxygen replacement with two fluorine atoms in conformationally hindered C=O systems, and (b) conversion of carboxylic acids into CF_3-containing products without sacrificing efficiency.
In this report, we will summarize over a decade of hands-on experience benchmarking SF_4 against DAST-type reagents. We will discuss internal decision criteria for reagent selection, highlight transformations effectively exclusive to SF_4 (carboxylic acids, β-ketoesters, hindered ketones), report unexpected protecting-group tolerance, and outline practical safety strategies for multigram-scale autoclave applications.

[1]Trofymchuk, S. A.; Kliukovskyi, D. V.; Semenov, S. V.; Khairulin, A. R.; Shevchenko, V. O.; Bugera, M. Y.; Tarasenko, K. V.; Volochnyuk, D. M.; Ryabukhin, S. V. *Synlett* **2020,** *31* (06), 565-574.
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MDR - D3 - F02

Mechanism elucidation of paddle-wheel di-Ru complex catalyzed amination reaction via multireference theory

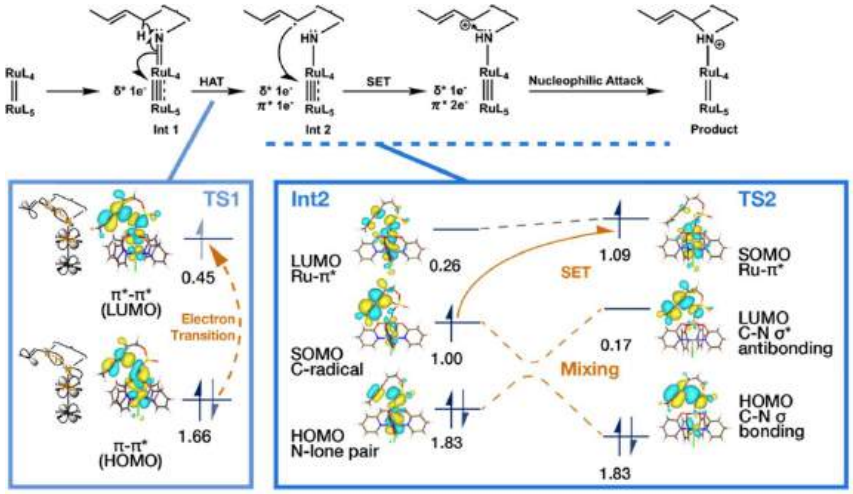
Maria Kosaka[1], Yuki Kurashige[1,2,3]
[1]Kyoto University, Japan; [2]CREST, Japan; [3]FOREST, Japan

Paddle-wheel dinuclear organometallic catalysts are of great interest, yet the system shows a strong multireference effect; thus, many issues on the electronic structure and the reaction mechanism have remained unclear. Here, we addressed the highly accurate calculation on the diRu catalytic C-H activation-amination, which consists of two steps: First, hydrogen atom transfer (HAT) from allyl C to the nitrene N in the nitrenoid intermediate (Int1); second, the C-N bond formation in the C-radical intermediate (Int2) to provide the ring amine (Product). Utilizing the multireference theory, the intermediates and the transition state structures were optimized, and the electronic structure was analyzed.

First, for the HAT step, the transition state (TS1) structure was searched based on the multireference theory. According to the analysis of the natural orbitals and the occupation numbers, the electron transition from the HOMO to the LUMO proceeds along the process, implying the mechanism as a concerted homolytic C-H, N-Ru cleavage and H-N bond formation. This radical reaction path is facilitated by the radical character shown at Int1 even before the reaction.

Second, for the annulation step, the electronic structure was analyzed on the transition state (TS2) structure optimized in the same manner as above. The mechanism is not a radical coupling; rather, the single electron transfer from the C-radical center to the unoccupied Ru-π* orbital in the Int2 species, followed by the nucleophilic attack from N to the carbocation.

In this way, the electronic structure of each species through the reaction was analyzed to reveal the catalytic reaction mechanism, utilizing the highly accurate electronic state theory.



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[2]K. Mori, et.al. *Bull. Chem. Soc. Japan*. **2025**, 98, 11, uoaf106.

MDR - D3 - F03
Ionic-group densification of perfluorinated high-oxygen-permeability ionomers

HunHee Han, Young-Je Kwark*
[1]*Dept. of Green Chemistry and Materials Engineering, Soongsil University, Seoul, Korea*

High-oxygen-permeability ionomers (HOPIs) for proton-exchange membrane fuel cells were prepared as copolymers of perfluoro(4-methyl-3,6-dioxaoct-7-ene) sulfonyl fluoride (PSEPVE) and perfluoro-2,2-dimethyl-1,3-dioxole (PDD). PSEPVE introduces sulfonic acid groups for ion conduction, whereas PDD enhances oxygen permeability. Optimizing membrane performance at a given ion-exchange capacity (IEC) requires control not only of the average PSEPVE/PDD ratio but also of the intrachain and interchain spatial distribution (local density) of ionic groups.

In sulfonated hydrocarbon polymer systems, many studies have shown that, at fixed IEC, block or blocky architectures exhibit higher proton conductivity and more continuous hydrated channels than purely random copolymers. These observations support the design principle that local clustering of ionic groups is more effective for forming ion-conducting channels than merely increasing their overall content.

Conventional free-radical copolymerization of PSEPVE and PDD produces statistical copolymers in which ionic groups are distributed rather uniformly along the chains and chain-to-chain compositions are broadly dispersed. Such structural randomness can hinder the formation of locally enriched ionic domains and continuous ion-conducting pathways, particularly at low ionic-group contents. To mitigate this, we employed reversible deactivation radical polymerization via the reversible addition–fragmentation chain-transfer (RAFT) mechanism. A fluorinated xanthate chain-transfer agent was used to ensure compatibility with the fluorinated monomers and to narrow the molecular-weight and composition distributions. The resulting HOPIs do not exhibit fully phase-separated block architectures but are designed to display increased local sulfonyl-group density. Copolymer composition, chain-structure uniformity, solution viscosity, and glass transition temperature for RAFT-derived HOPIs were compared with those of materials prepared by conventional free-radical polymerization to evaluate how RAFT-based chain-structure control facilitates the formation of effective ion-conducting channels at relatively low ionic-group loadings.

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MDR - D3 - F04
Strapped Calix[4]pyrroles for the transmembrane transport of anions

Priyanka Rani Panda, Karolis Norvaisa, and Hennie Valkenier
Engineering of Molecular NanoSystems, Université Libre de Bruxelles, Belgium

Maintaining cellular homeostasis in our body is crucial for physiological processes regulated by the transport of molecules across cell membranes via simple diffusion of small, uncharged molecules and facilitated diffusion of charged species and polar molecules by ion channels or carriers.[1] Synthetic transporters are molecules that mimic the biological ion transport process. Thus, a wide variety of molecular scaffolds have been designed to target specific ions of interest.[2] For example, calix[4]pyrrole is a widely explored moiety in anion recognition chemistry and has shown promising results as synthetic transporter in lipid bilayers. It forms a bowl-shaped cavity comprising four pyrrole units linked by methylene bridges, which can be functionalised with straps and walls with additional binding motifs to enhance ion binding affinity, preorganization and the transport activity.[3] In 2023, our group reported a bisurea-strapped calix[4]pyrrole **1** as the first synthetic phosphate transporter, overcoming the high hydration energy barrier to effectively transport phosphate across the lipid bilayer.[4] Building on this previous work, a series of strapped calix[4]pyrroles with varying receptor properties (i.e., cavity size and the number of hydrogen-bond donors) has been synthesised to address the following research questions: First, how do the variations impact phosphate transport and to what extent the cavity size and HB donor points can be reduced to observe phosphate transport activity? Second, how do subtle changes in receptor design affect the transport selectivity of other anions of different size and hydration energies (i.e., Cl^-, NO_3^-, Br^-, I^-, ClO_4^-)? Herein, we present the transport activity and selectivity trends in the strapped calix[4]pyrrole systems.

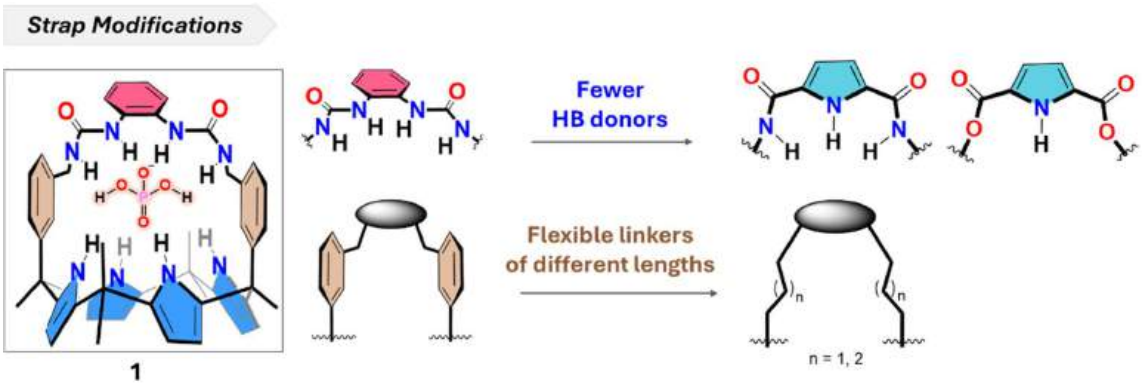

Fig. 1. Schematic of the structural modifications introduced to the design of transporter **1.**

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[2]Gale, P. A. et al. ; *Chem. Soc. Rev.* **2017**, *46*, 2497–2519.
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MDR - D4 - O01
Effect of the directionality of the external force on the rupture of mechanophores

Shouryo Ghose, Francoise Remacle
Theoretical Physical Chemistry, Research Unit MOLSYS, University of Liège, Belgium

Polymeric materials containing weak sacrificial bonds can be designed to engineer self−healing, higher toughness, and improve melt−processing. However, they usually exhibit a lower mechanical strength and are subject to creep and fatigue. For improving their design, it is of interest to investigate their mechanical response at the atomic and molecular scale.
We investigate computationally the effect of the directionality of the force on mechanophores keeping the modulus of the force constant.There are several ways to break the mechanophore since there are more than one bond to break. We show that it is not necessarily the modulus of the force that determines the rupture, rather it is its directionality. In particular, for a given modulus of the applied force vector, exerting a torque on the adduct can lead to rupture at a lower force than applying the force in a direction parallel to the targeted bonds[3]. We investigate two adducts with weak dynamic covalent bonds, the Zinc-Bis-Terpyridine complex and the Furan-Maleimide molecule.The external force is modeled using a dynamical “AISMD”[1] approach where a constant external force is applied to the pulling atoms in the direction of the laboratory attached fix points (see Fig 1).The effect of solvent (DMSO) is also considered. We discuss the dynamics of bond rupture and of the redistribution of the energy provided by the external force over the complex through the analysis of the structural changes and of the evolution of potential and kinetic energy as a function of time.We also analyze the recombination processes after the bond ruptures[2].

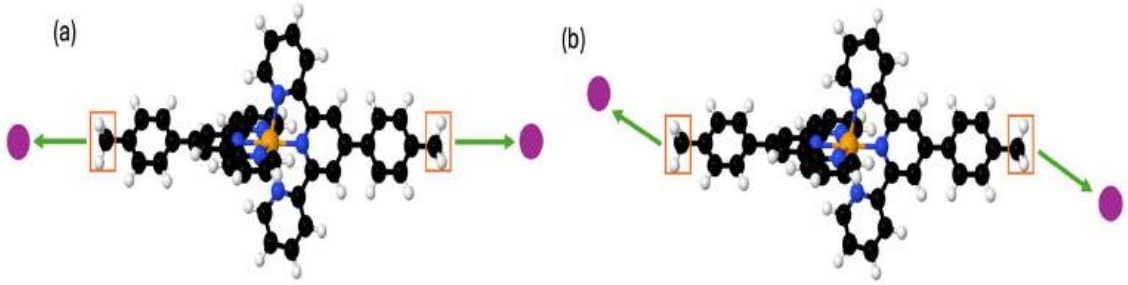

Fig. 1. Schematic representation of the pulling points and steering atoms for AISMD of the [Zn-bis-terpy]+2 mechanophore. Two different directions of the pulling are shown in panel (a) and (b) respectively. In both cases the pulling atoms are the C of the two terminal CH_3 groups (marked in orange box) and the fixed points are marked in violet circle.

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MDR - D4 - O02
Write and erase: Macrocyclic effectors regulate imine expression in water

Ferran Esteve[1,*], Martina Mazzaferro[1,2,3], Jean-Marie Lehn[1]
[1]Laboratoire de Chimie Supramoléculaire, Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Université de Strasbourg, France; [2]Dipto di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, Università degli Studi di Messina, Italy; [3]Dipto di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Italy

Protein post-translational modifications (PTMs)[1] are enzymatically reversible reactions that temporarily/locally switch protein structure, dynamics, interaction and function.[2] This dynamic process involves the selective action of three groups of enzymes: a *writer* promoting the PTM, a *reader* recognizing the modification and triggering the assigned pathway, and an *eraser* reversing the transformation.[3] We envisaged that a related mechanism of regulation could be attained by exploiting the reversible nature of host:guest and dynamic covalent chemistry.[4] Imine formation reactions are considered since they rely on amine modification and resemble natural PTMs on lysine residues (Lys).[5]
The introduction of a macrocyclic compound with a preorganized cavity (*i.e., writer*) that can selectively recognize a specific species of a dynamic covalent reaction modulates the overall thermodynamic profile and shifts the equilibrium accordingly (*i.e., information processing*). Addition of a better guest (*i.e., eraser*) for the *writer* scavenges the macrocycle effect and restores the initial equilibrium state of the reaction.[6]
This synthetic strategy allows for the emergence of *complex behavior* like (non)selective *up-* and *down-regulations*, *constituent selection*, *selectivity switching* and *sorting-to-scrambling* transitions. Its implementation in dynamic libraries of model peptidomimetics opens new avenues in the effector-driven reversible modification of biomolecules with tunable site-selectivity.

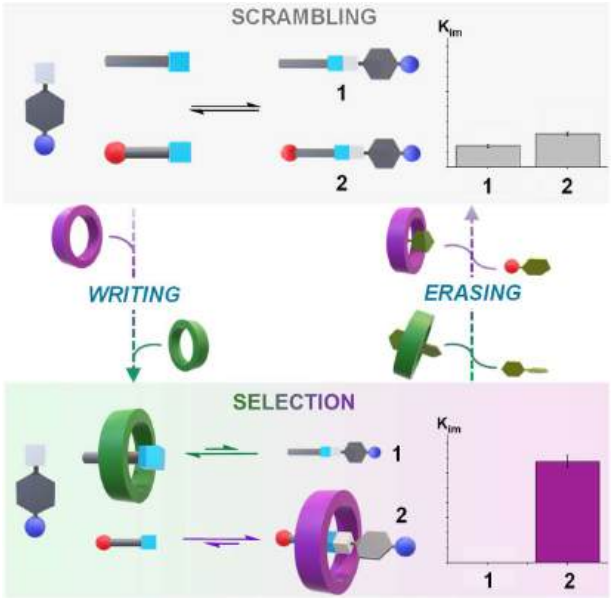

Fig. 1. Example of *complex behavior* emergence within a dynamic covalent library.

This work was supported by the Agence Nationale de la Recherche in France (ANR-20CE07-0031), University of Strasbourg Institute for Advanced Study, and Fondation Jean-Marie Lehn. This project has also received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 101151945.

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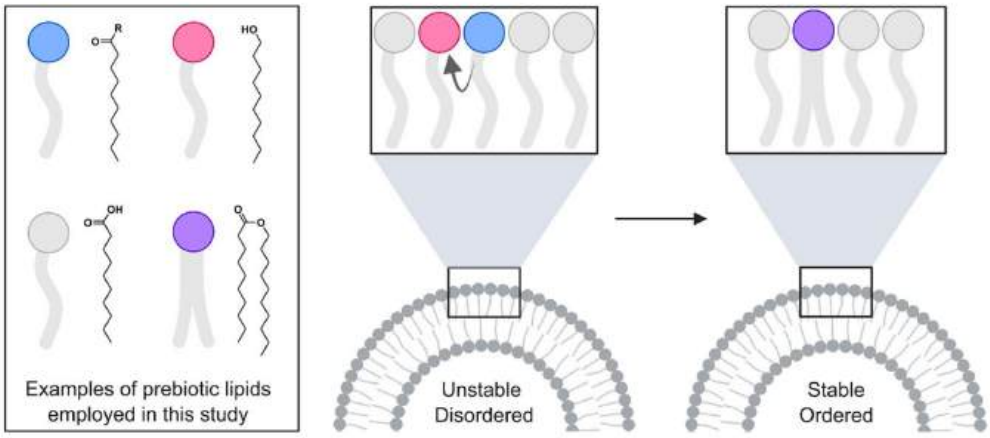
MDR - D4 - O03
A novel prebiotic pathway for lipid acylation

Fidan Rahmatova[1,2], David A. Russell[1], Claudia Bonfio[1]
[1]Dept. of Biochemistry, University of Cambridge, UK; [2]Institut de Science et d'Ingénierie Supramoléculaires (ISIS), University of Strasbourg, France

The emergence of protometabolism on early Earth required prebiotically plausible pathways to synthesize and modify key biomolecules, including lipids. Inspired by pioneering work demonstrating the self-assembly-driven non-enzymatic synthesis of natural phosphatidylcholines,[1] we show that primitive membranes can similarly facilitate acylation reactions at neutral pH, using acyl imidazoles as efficient, prebiotically relevant acylating agents.[2] We demonstrate the efficient acylation *in membrana* of diverse prebiotic substrates, including lysophospholipids with different headgroups,[3] monoester/ether glycerols, and alcohols of varying chain lengths. By employing primitive membranes as both reaction templates and organizational scaffolds, we reveal a potential pathway for prebiotic acyl-group transfer, driven by chemical reactivity rather than enzymatic control, which could have mimicked early biochemical steps toward protocell membrane diversification. Our findings bridge non-enzymatic synthesis on a large library of substrates with primitive membrane-mediated chemistry, offering insights into how spontaneous chemical processes might have led to the functional complexity of early cells.



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MDR - D4 - O04
Synthesis of amphiphilic pyrene–BODIPY sulfonates with self-assembling properties

M. Cordaro[1], G. Neri[1], M. Trapani[2], A. Arrigo[1], A. Santoro[1], A. Piperno[1]
[1]Dip. CHIBIOFARAM, University of Messina, Italy; [2]CNR- ISMN c/o Dip. CHIBIOFARAM, Università di Messina, Italy

Self-assembly processes provide a powerful tool for the synthesis of nanostructures with tailored properties. Here, amphiphilic BODIPY fluorophores bearing pyrene and styryl sulfonates have been designed to couple water solubility with cell membrane permeability. The probes form nanoaggregates in aqueous media and show a red-shifted emission. Spectroscopic studies reveal an efficient energy transfer from pyrene donor subunit to the BODIPY acceptor and an extended conjugation from styryl units. Probes have been synthesized via Knoevenagel condensation on the BODIPY core[1] to introduce styryl units, followed by sulfonation with propanesultone under basic conditions (Figure 1).
The sulfonate groups allow the water solubility while the pyrene unit can enable π–π stacking interactions for a potential integration with graphene and carbon surfaces for signal amplification and surface readouts.[2] Because the BODIPY core is readily post-functionalized, emission and affinity can be tuned without losing amphiphilicity, allowing task-specific variants.
Overall, these amphiphilic pyrene–BODIPY sulfonates provide a compact and tunable platform that combine self-assembly in solution with reliable cellular imaging and sensor design. They are straightforward to prepare, work at low concentrations, and can be adapted to workflows in imaging, microfluidic assays, and material-integrated biosensors.[3]

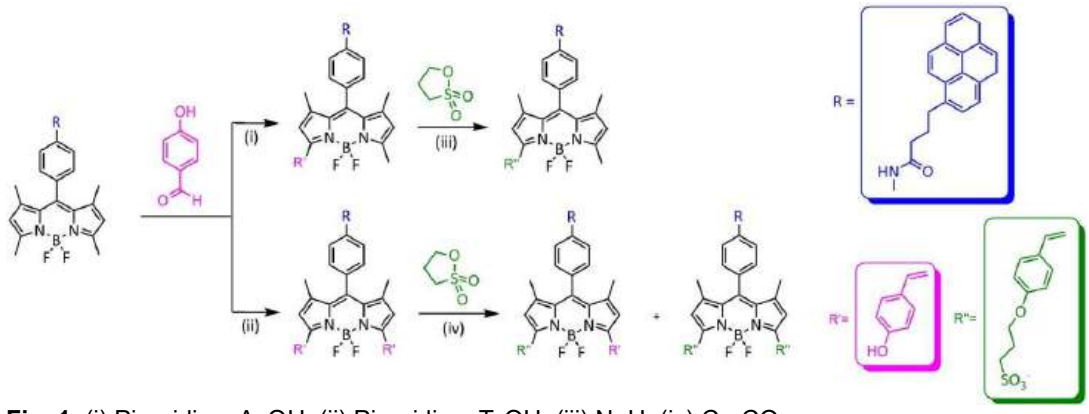

Fig. 1. (i) Piperidine, AcOH; (ii) Piperidine, TsOH; (iii) NaH; (iv) Cs_2CO_3.

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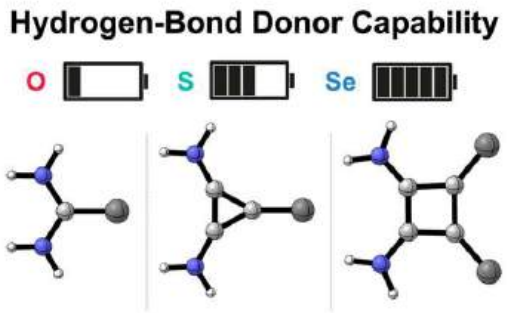
MDR - D4 - O05
Effect of chalcogen atom size on hydrogen bond strength in chalcoamide-based linear polymers

Siebe Lekanne Deprez[1], Lucas de Avezedo Santos, Celine Nieuwland[1], Pascal Vermeeren[1], Célia Fonseca Guerra[1]
[1]*Vrije universiteit Amsterdam, The Netherlands*

Why do some supramolecular building blocks form stronger chains than others? We explored this question by zooming in on urea, deltamide, squaramide, and their sulfur and selenium analogs (chalcogens) – all common building blocks in supramolecular chemistry. Experimental work indicates considerable structural differences in hydrogen bonding upon interchanging oxygen by its heavier relatives. Using relativistic, dispersion-corrected DFT, we discovered that larger chalcogens make better hydrogen-bond donors.[1-4] As the chalcogen size increases, the larger chalcogen withdraws more charge from adjacent amino groups, amplifying the positive character of hydrogen donors and strengthening their interaction with negatively charged acceptors.



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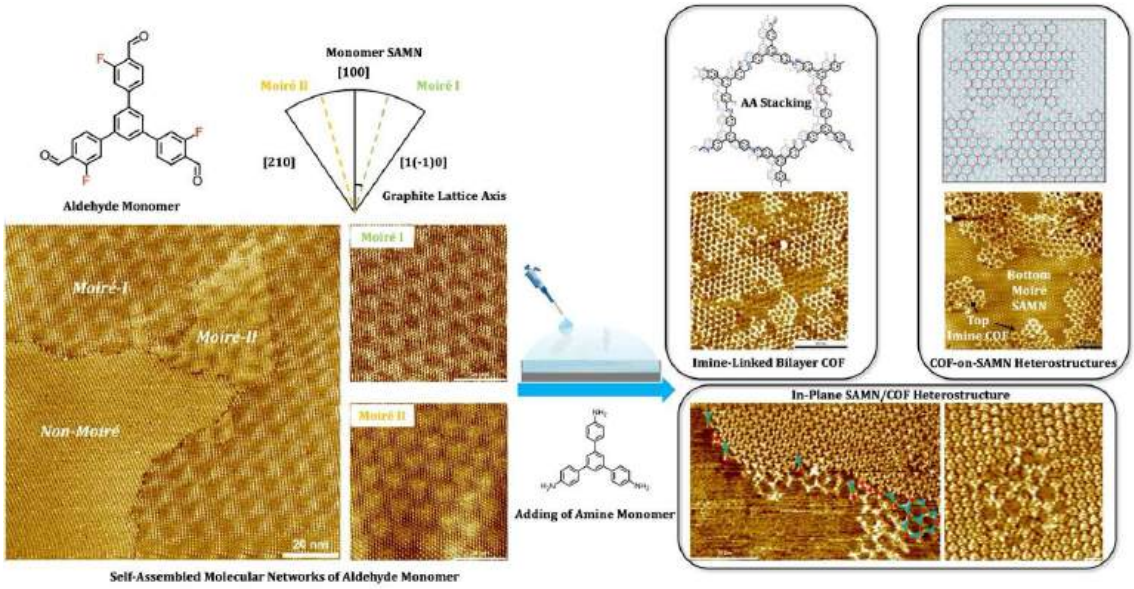
MDR - D4 - O06

Design of controllable two-dimensional heterojunction structures on surfaces - Starting from moiré self-assembled molecular networks

Jie Zhang[1], Steven De Feyter[1]
[1]*Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Belgium*

Surface/interface chemistry provides a route to reveal molecular-level mechanisms. In the solvothermal or microwave-assisted syntheses of imine-linked covalent organic frameworks (COFs), the processes of monomer preorganization, diffusion, and early growth are challenging to resolve due to the limited in situ characterization and the complex, rapidly evolving reaction pathways.[1–3] In parallel, moiré materials arising from lattice mismatch or rotational misalignment in 2D layers have attracted great interest, yet the moiré superlattice and its impact on adsorption and epitaxy remain poorly understood. In this contribution, we build a 2D model platform on a graphite surface, where fluorinated aldehydes form densely packed self-assembled molecular networks (SAMNs) featuring three orientationally distinct domains (non-Moiré, Moiré-I, and Moiré-II). By programming the Schiff-base reaction upon amine introduction, we steer on-surface polymerization into three discrete hybrid architectures: **imine-linked bilayer COFs**, **in-plane SAMN/COF heterostructures**, and **COF-on-SAMN hetero-bilayers**. Notably, the in-plane pathway exhibits kinetic trapping that arrests early nucleation events, enabling STM imaging of the growth process and revealing previously inaccessible nanoscale intermediate motifs. More importantly, these observations demonstrate a switchable Moiré SAMN interface that toggles between a **reactive precursor state** (in-plane conversion) and a **passivating template state** (heterostructure growth), yielding SAMN - COF interfaces in both lateral and vertical geometries. Beyond creating new bilayer heterostructures, this platform will isolate how preorganization and kinetic arrest dictate registry, stacking, and defect evolution, providing mechanistic design rules to bulk COF synthesis.



Acknowledgements: This work is supported by the European Union under the Horizon Europe grant 101046231 (FantastiCOF) and by M-ERA.NET (SuperSuper) call via FWO project G0K9822N. KU Leuven–Internal Funds (C14/19/079) is acknowledged.

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MDR - D4 - O07
Nanotube-induced organic frameworks (N_IOFs) via a topochemical reactions

Javed Pathan, Kristof Van Hecke
Ghent University, Belgium

Organic nanotubes (ONTs)[1] and organic framework materials, including covalent organic frameworks (COFs),[2] hydrogen-bonded organic frameworks (HOFs),[3] and metal-organic frameworks (MOFs),[4] possess well-defined architectures, tunable chemical functionalities, and inherent biocompatibility. These features make them promising candidates for applications in molecular transport, catalysis, sensing, energy storage, and nanomedicine. However, conventional solution-phase synthesis often yields materials with poor crystallinity, limited scalability, and weak structural control, obscuring clear structure–property relationships. Topochemical polymerization overcomes these challenges by exploiting preorganized arrangement of reactive building blocks within single crystals to form covalent bonds under mild, solvent- and catalyst-free conditions.[4]
We aim to extend this excellent strategy toward the synthesis of a new class of porous materials. Specifically, we propose nanotube-induced organic frameworks (N_IOFs), an unexplored materials platform generated through topochemical reactions. By integrating organic nanotubes within hydrogen-bonded organic frameworks, this approach combines the advantages of both components within a single crystalline system. The resulting structures are expected to exhibit dual porosity, arising from the intrinsic channels of the nanotubes and the extrinsic pores of the surrounding framework, thereby enabling multifunctional behavior. By leveraging expertise in supramolecular chemistry, solid-state polymerization, and crystal engineering, this research seeks to establish a robust solid-state platform for the controlled synthesis of N_IOF with tunable structures and functions.

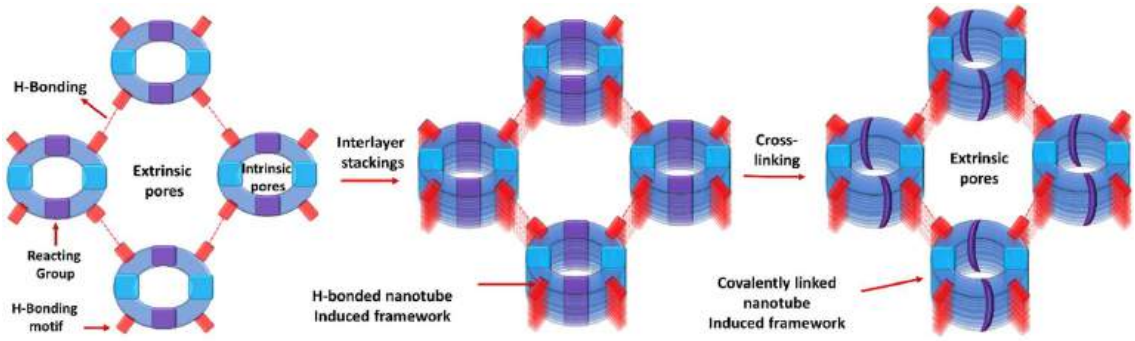

Fig. 1. Schematic representation of covalently linked N_IOF via topochemical reactions.

Acknowledgement: JP and KVH thank the Special Research Fund (BOF) – UGent (Project: bof/baf/4y/2024/01/214).

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MDR - D4 - O08
Artificial phototactic microswimmers for precise light-guided navigation

Angie Bolaños[1], Majid Basharat[1], Shang Gao[1], Katherine Villa[1,2]
[1]Institute of Chemical Research of Catalonia (ICIQ), Spain; [2]Institució Catalana de Recerca i Estudis Avançats (ICREA), Spain

Phototaxis, the directional response of organisms to light, has inspired artificial light-driven microswimmers[1]. Steerable microswimmers with precise light-induced motion promise applications in drug delivery, cargo transport, environmental remediation, and artificial life-like systems. However, most photoactive microswimmers display random trajectories and limited steering, often requiring multicomponent designs[2] or external magnetic or electric fields[3], which increase system complexity and hinder precise control of direction and velocity.
Here, we report single-component photocatalytic microswimmers synthesized by a hydrothermal reaction. Their motion is driven by photoinduced chemical reaction, enabled by efficient charge separation at a surface heterojunction between distinct crystallographic facets[4]. Under structured light fields, the microswimmers exhibit phototaxis, sensing and migrating toward illuminated regions. Using static and dynamic light patterns generated by a digital micromirror device (DMD), we achieve programmable control over trajectories, velocity modulation, and spatial confinement with precision. This strategy enables simultaneous independent manipulation of multiple microswimmers. Owing to its minimal system complexity and rapid adaptability to changing illumination patterns, this light-guided approach provides a versatile platform for directing microswimmer motion. These results represent an important step toward the realization of adaptive and autonomous microsystems that mimic key functionalities of biological phototactic organisms.

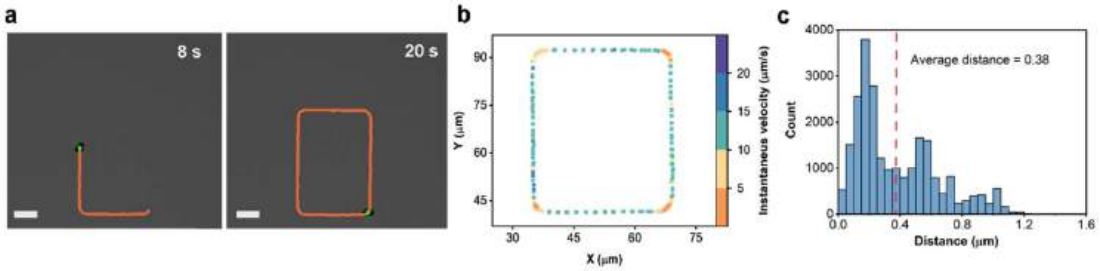

Fig. 1. (a) Trajectory of the microswimmer motion around a static rectangular light pattern. (b) Instantaneous velocity at each point along the trajectory. (c) Frequency distribution of the deviation between the microswimmer trajectory and the light pattern. All scale bars correspond to 10 μm.

The research was funded by the European Union (ERC, PhotoSwim, 101076680). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them. This publication is part of the grant CNS2024-154696 financed by MICIU/AEI/10.13039/501100011033.

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MDR - D4 - O09
Development of synthetic transmembrane transporters for phosphates

Karolis Norvaisa[1], Priyanka Rani Panda[1], Aaron Torres-Huerta[1], Uththara M.C. Rathnaweera[2], Nathalie Busschaert[2], Stephen J. Butler[3], Hennie Valkenier[1]
[1]Université libre de Bruxelles (ULB), Belgium; [2]Tulane University, USA; [3]Loughborough University Institution, UK

Phosphates and phosphorylated compounds play essential roles in biological processes, including energy transfer (e.g., ATP) and enzymatic activity (e.g., RNA and DNA polymerases).[1] Many biosensors have been developed for key metabolites such as NADPH, NAD^+/NADH, ATP, and phosphorylated glycolytic intermediates.[2] However, the anionic and highly hydrophilic nature of phosphorylated metabolites prevents passive diffusion across cell membranes, necessitating specialised transport proteins. Despite their biological importance, synthetic systems capable of transporting phosphate derivatives remain scarce, although notable advances have been reported.
Previously, we have demonstrated that a strapped calix[4]pyrrole can facilitate the transmembrane transport of the highly hydrated $H_2PO_4^-$,[3] and more recently that a two-component small-molecule transport system enables the transport of cAMP and AMP.[4]
Here, we present a systematic study of phosphate and phosphate ester transport using synthetic anionophores.[5] Transport into liposomes was monitored by fluorescence and ^{31}P NMR spectroscopy. Our results highlight the critical role of pre-organized molecular frameworks with multiple hydrogen-bonding sites in facilitating inorganic phosphate transport, whereas simpler carriers are more effective for less hydrated, lipophilic phosphate esters. These findings provide key insights into design principles for synthetic anionophores targeting biologically relevant phosphate species.

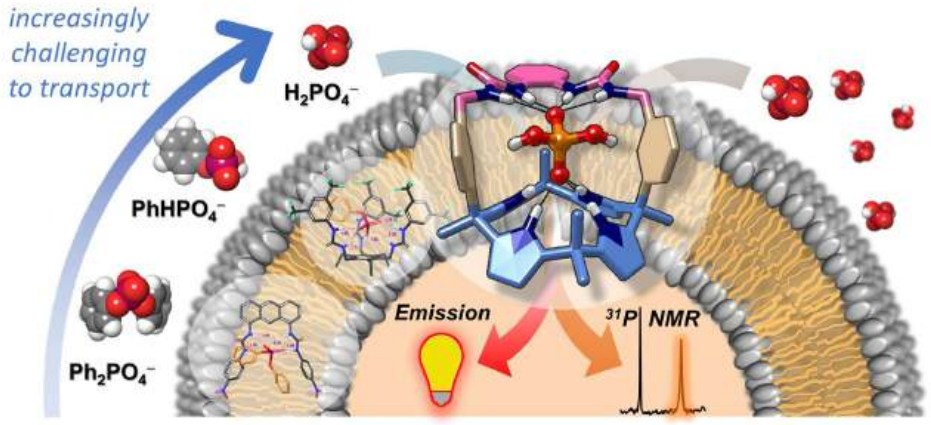

Fig. 1. Graphical representation of phosphate species transported into liposomes by various anionophores, monitored using two complementary assay methods.

This project has received funding from the European Research Council (ERC, Grant agreement No. 802727) and the Walloon region through the Fonds de la Recherche Scientifique – FNRS. This communication is based upon the work from COST Action LUCES CA22131, supported by COST (European Cooperation in Science and Technology).

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MDR - D4 - O10
Ru(II)-peptide conjugates for photoactivated chemotherapy

Irene Regeni[1], Marouscha Puister[2], Sylvestre Bonnet [2]*
[1]Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Strasbourg University, France; [2]Leiden Institute of Chemistry, Leiden University, The Netherlands

Nature-derived anticancer peptides (ACPs) such as Mastoparan X and Halictine display potent cytotoxicity through disruption of cancer cell membranes. When folded into their characteristic α-helical secondary structures, these peptides adopt amphipathic topologies that drive their interaction and insertion into lipid bilayers, ultimately forming transient pores. Despite their promise, clinical translation remains constrained by heavy side effects caused by off-target membranolysis and rapid enzymatic degradation.
Here, we present a light-activated strategy to regulate ACPs' bioactivity with high spatial precision. ACPs are temporarily deactivated through coordination to ruthenium(II) polypyridyl complexes,[1] which perturb helix formation and attenuate the peptides' membrane-binding interface. Upon irradiation with visible light, photoinduced ligand dissociation releases the native peptide, restoring its supramolecular membrane-disruptive function on demand. This metal-mediated caging approach enables control over peptide folding and membrane interaction, offering a generalizable platform for precision-activated peptide therapeutics.[2]

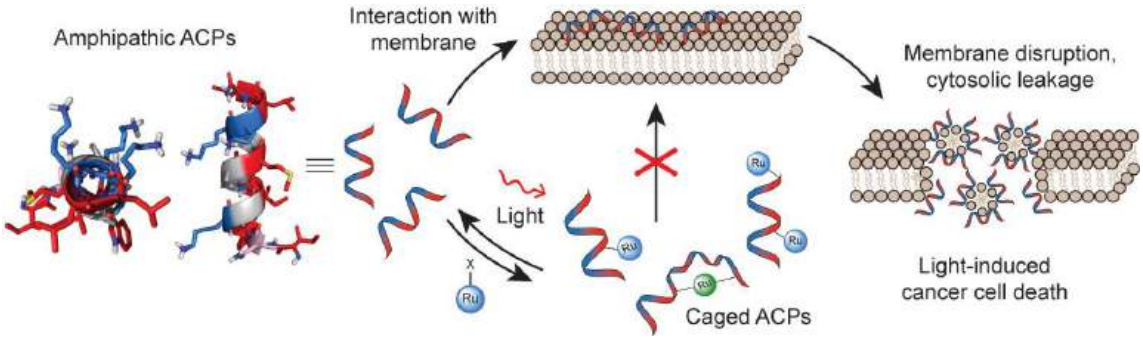

Fig. 1. The amphipathic peptide Mastoparan X (PDB ID: 2CZP) strongly interacts with cell membranes and self-assembles into pores that induce cell death. In contrast, the peptide caged with Ru(II) polypyridyl complexes is unable to interact with the membrane. Upon light irradiation, ligand substitution cleaves the Ru–peptide coordination bond, restoring the peptide's membrane-disrupting activity.

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MDR - D4 - O11

Second-coordination sphere of pyrazoles metal complexes: From anion recognition to bimetallic assemblies

Corentin Pochet[1], Tristan Laurent[2], Michael L. Singleton[2]
[1]Laboratory of Organic Electronics, ITN, Linköping University, Sweden; [2]MOST, IMCN, UCLouvain, Belgium

Second-coordination sphere refers to interactions, mainly non-covalent, between a metal complex and its environment. These interactions play a crucial role in the properties and reactivity of coordination complexes making them important for a range of applications including sensing and catalysis.[1] Controlling and predicting the second-coordination sphere relies on the precise placement and orientation of these interactions which depends on the metal ion's geometric preferences and the nature of the ligand scaffold.

In this respect, hexadentate ligands, especially TPEN-based, offer a robust and tunable platform for integrating and controlling the placement of second coordination sphere interactions due to the stability and predictability of their coordination compounds.[2,3] In 2018, our group modified the TPEN scaffold by introducing pyridazine moieties to add secondary binding sites.[4] The additional endocyclic nitrogen atoms act cooperatively to bind protons, thereby preventing decomplexation of Fe^{II} complexes in highly acidic media. Despite highlighting promising perspectives, our pyridazine systems remain limited to interact with protons.

To extend the range of possible interactions, switching from pyridazine to pyrazole inverts the polarity of the interaction site and allow binding to anions instead. Moreover, the acidic N-H groups of the pyrazoles are available for deprotonation, tuning the redox properties of the metal centres and reforming a suitable binding site for cationic species. Last year, we reported the ability of a first series of pyrazole-based metal complexes to bind anions (Figure 1).[5]

Now, the expanded scope and tunability of our systems afford a new series of pyrazole-based complexes that function as moderately to highly sensitive anion receptors, redox modulators of the metal centres, and versatile precursors to bimetallic architectures relevant to catalysis.

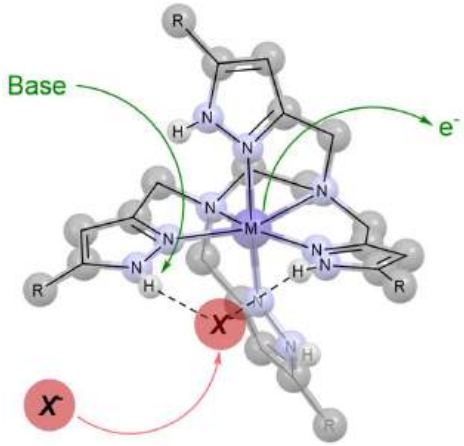

Fig. 2. Schematic pyrazole-based metal complexes as anion receptors or redox modulator.

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The 10th EuChemS Chemistry Congress

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Responsible Chemistry (RC)

RC - D1 - O01

Equipping future chemists for societal challenges: Integrating ethics and interdisciplinarity in materials science

Dorien Baeten[1], Sarah Doumen[1], Geert-Jan Graulus[1,2], An Hardy[1,2]
[1]Faculty of Sciences, Hasselt University, Belgium; [2]Institute for Materials Research, Hasselt University, Belgium

The urgent need to address complex challenges, such as climate change, an aging population, and the energy transition, requires chemists who can exceed traditional disciplinary boundaries and act with ethical accountability. To achieve this, our materials science master's program prioritizes interdisciplinary learning via an integrated learning line that builds on the learning mechanisms proposed by the boundary-crossing theory: identification, coordination, reflection, and transformation[1]. Each course within the curriculum is required to explicitly state which mechanism(s) are addressed.

This contribution focuses specifically on the two advanced mechanisms of this framework: reflection and transformation. We detail specific teaching and assessment methods (e.g., interdisciplinary projects and other active teaching methods, such as debates) employed to foster these competencies. Additionally, we discuss how teachers and students experience this integration. These results originate from a Design-Based Research study focused on monitoring and refining this interdisciplinary education.

We also further highlight how students strengthen their reflection and transformation competencies through the dedicated course Capita Selecta. In this course, students are repeatedly challenged to review their perspective on their education and research based on stakeholder insights. Students reflect, often in interaction with external experts, on their own activities and future ambitions through contributions focusing on applied ethics, innovation management, intellectual property rights, science communication, and science governance. This pushes them toward ‘transformation’, enabling them to adapt their practice and integrate ethical, societal, and ecological considerations into their problem-solving methodology.

This contribution aims to inspire educators and program directors by demonstrating how interdisciplinary learning and a dedicated course can effectively equip graduating scientists with the necessary competencies to address societal challenges in a responsible and ethical manner.

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RC - D1 - O02
The Da Vinci master programme: Educating sustainability change-makers

Fieke Sluijs[1], Eelco Vogt[1], Bert Weckhuysen[1], Sabine Uijl[2]
[1]Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry (ISCC), Dept. of Chemistry, Faculty of Science, Utrecht University, The Netherlands; [2]Research group Studies of Interdisciplinary Learning and Teaching (SILT), Institute for Cultural Inquiry (ICON), Faculty of Humanities, Utrecht University, The Netherlands

Chemistry has the potential to play a key role in the transition towards a more sustainable and circular society, but to maximize its potential, far-reaching changes are needed in chemical industry, politics, research, and education, including chemistry curricula.[1-6] Research has shown that incremental technical innovation is insufficient for a transition towards a sustainable chemical industry, since it requires large-scale disruptive changes in sociotechnical systems.[7-10] Interventions in socio-technical systems call for long-term strategic collaboration underpinned by a firm commitment from the scientific community, industry, finance, and policymakers.[11-14] Hence, there is a strong demand for chemistry professionals in all these domains that can contribute to successful systemic interventions, individuals with profound knowledge of sustainable chemistry, including systems thinking, as well as resilient intra- and inter-personal abilities. In educational research on the Da Vinci Project, we discovered that students develop crucial competencies to drive sustainability transitions,[15] as shown in figure 1c.
This presentation highlights our educational design research on the **Da Vinci Master Programme 2026** at the Institute for Sustainable and Circular Chemistry (ISCC), Utrecht University. Following up on the success of the Da Vinci Project for bachelor students, the Da Vinci Master Programme has been developed as a transdisciplinary challenge-based learning experience to enable master students from three Dutch universities (TU/e, WU, UU) to develop sustainability change-maker competencies. The programme is a 20-week full-time learning journey in which interdisciplinary teams work on complex real-life sustainability challenges in collaboration with societal partners. Students are trained in systems thinking, design thinking and interdisciplinary research to apply these approaches while iteratively exploring the challenge and developing solutions. They work three days a week at a societal partner to access the non-academic network and optimize co-learning of stakeholders. Figure 1a shows the pedagogical approach of Da Vinci and 1b shows the iterative approach to tackle the challenge.

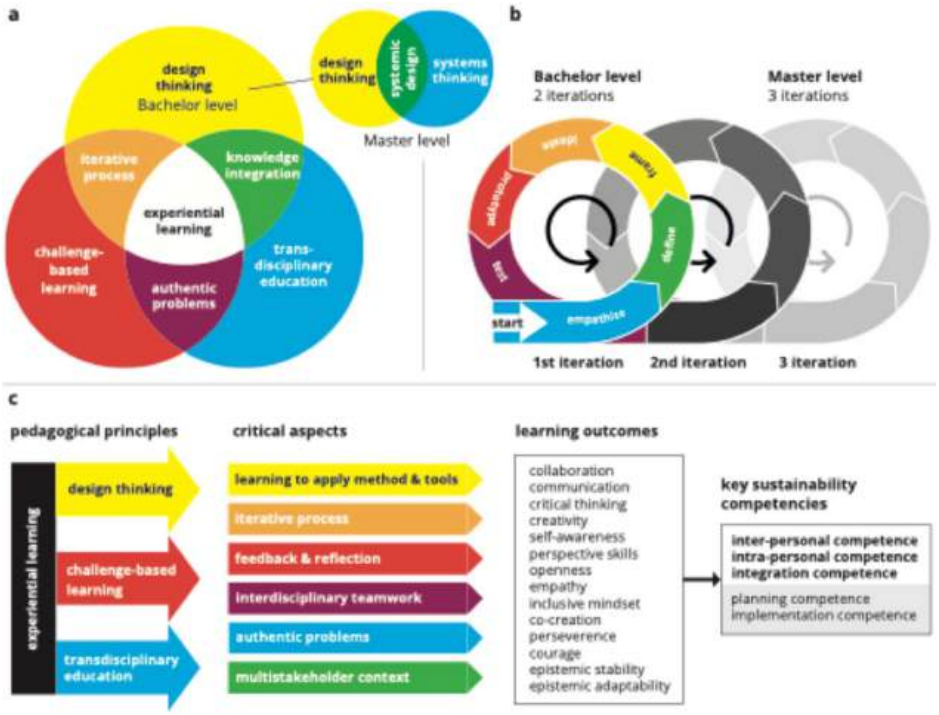

Fig. 1. (a) Pedagogical principles of the Da Vinci Project: students work in interdisciplinary teams, tackling authentic sustainability challenges (challenge-based learning), in collaboration with non-academic stakeholders (transdisciplinary), applying design thinking methodology and tools for integrative problem-solving. Integrative problem-solving requires integration of knowledge from multiple disciplines and of

theoretical and practical knowledge. Challenge-based learning and design thinking are iterative processes. These pedagogical principles are descent from experiential learning theory in which learners go through multiple cycles of four modes of learning: concrete experience, reflective observation, abstract conceptualization, and active experimentation. This cyclic process coincides with the design cycles. (b) In the Da Vinci Project (Bachelor level) fulfil two iterations, applying the stages from the Stanford d.School model. Students in the Da Vinci Master Program fulfil three iterations, applying a more advanced systemic design process of which the steps are not shown here. (c) Overview of how the pedagogical principles foster sustainability competency development in the Da Vinci Project, based on Sluijs et al.[15] Certain critical aspects of the pedagogical principles enable specific learning outcomes that are related to key competencies for sustainability. In the Da Vinci Project, interpersonal, intrapersonal, and integration competencies are clearly recognized in the learning outcomes. The two other key competencies (grey area) are recognized as learning outcomes, but not as clearly.

More information on the Da Vinci Project and the Da Vinci Master Programme

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- C2W interview in Refinery of the Future: https://www.sciencelink.net/refinery-of-the-future/becoming-a-21st-century-chemist/22378.article
- Website Da Vinci Project: https://davinciproject.nl/
- Information on Da Vinci Programme for students: https://ewuu.nl/en/education/challenges/the-da-vinci-programme-2026/

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RC - D1 - O03

Cultivating responsible chemists: The green chemistry commitment as a catalyst for educational systemic change

Juliana Vidal[1], Michelle Duarte[1], Omar Villanueva[1], Amy Cannon[1]
[1]*Beyond Benign Incorporated, USA*

The integration of green chemistry across the education continuum is essential to providing a long-lasting change towards a more sustainable future that addresses shared global environmental, health, and societal challenges. This approach can promote the development of scientists with the required skills to design safer products and processes for human health and the environment across diverse regional, cultural, and economic contexts worldwide. Furthermore, due to its intrinsic integrative nature, green chemistry education aligns with several of the internationally recognized Guiding Principles of Responsible Chemistry,[1] since it encourages sustainable and responsible innovation, implements a culture of safety, and promotes collaboration across disciplines to address our global challenges.

To catalyze the adoption of green chemistry in higher education settings, a non-profit organization known as Beyond Benign launched its Green Chemistry Commitment (GCC) program in 2013. The GCC is a commitment by universities, colleges, institutes, and centers worldwide to progressively work in the inclusion of green chemistry in their courses and curricula.[2] With over 260 participating institutions in more than 35 countries, this program has become a collective voice to drive systemic and behavioral change in chemistry education at the molecular level. In this presentation, diverse approaches used by higher education institutions across different national and regional contexts to integrate green chemistry through the GCC will be discussed, as well as the impact of the program in cultivating the next generation of responsible chemists.

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RC - D1 - O04
Q-method as a tool for transdisciplinary dialogue, reflexivity and learning in responsible chemistry

Sanghamitra Chakravarty[1], Gadi Rothenberg[1], Amanda Garcia[1]
[1]*Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands*

This paper discusses the use of Q-method as a tool to foster transdisciplinary dialogues, reflexivity and learning in responsible chemistry. It draws on our experience resulting from an interdisciplinary collaboration between a social scientist and chemists to investigate expectations around carbon dioxide electrochemistry in northwestern Europe using this method. Q-method is a mixed method used to study subjectivity in a complex topic in a structured manner combining statistical analysis and qualitative interview data. It consists of forced ranking of a set of statements representing all the viewpoints on a topic onto a grid, followed by an interview to understand the reasons behind the ranking. In our study, the Q-method was adapted to incorporate statements on social, ethical and sustainability aspects to anticipate socio-technical futures and applied in different settings including individual interviews, classroom and a workshop. Our research design also draws inspiration from a card-based methodology for public engagement rooted in science and technology studies by Ulrike Felt and colleagues. While technologies are shaped by a complex interplay of economic, social, cultural, political and contextual factors, disciplinary organisation of science, education and research makes understanding these interconnections which go beyond one's own discipline difficult. The Q-method was found to be an effective way of holistically thinking about social and ethical questions including provocative issues in a relatively conflict free manner. The quantitative aspect which involves factor analysis is received by some as a more credible alternative to only qualitative data. For the qualitative researcher, it offers a way of prioritising some key parameters influencing sociotechnical futures while not submitting to full reductionism. In this way, it could help bridge methodological divides. We conclude with reflections on how the Q-method can be adapted as a tool to foster transdisciplinary research and learning in responsible chemistry, while maintaining its methodological rigour.

RC - D1 - O06
SSbD as an anticipatory effort: The quest for a better future with chemicals

Jesse de Pagter[1,2]
[1]Centre for Social Innovation, Austria; [2]Technical University of Vienna, Austria

Across Europe, growing scrutiny of 'forever chemicals' such as PFAS has become an important driver of intensified calls for more sustainable chemical development. In parallel, within EU policy frameworks and industrial strategies, the principle of Safe and Sustainable by Design (SSbD) plays an important role in terms of guiding such transitions. This contribution foregrounds SSbD's anticipatory component: the notion that safety, sustainability, and broader societal concerns should be addressed early enough to shape research trajectories, design choices, and downstream value-chain options, rather than being treated as late-stage constraints.[1]

To contextualise this anticipatory orientation, the contribution first situates SSbD within a longer historical trajectory of chemical regulation and governance, highlighting a shift from reactive control toward more proactive, forward-looking approaches. It argues that anticipatory responsible innovation in the chemical domain requires an integrated, interdisciplinary approach that unites technical excellence with social responsiveness.[2] Subsequently, the contribution builds on insights from the EU-funded BIO-SUSHY project, which develops bio-based alternatives to PFAS-based coatings. Based on that, it illustrates how anticipation needs to become enacted through concrete methodological and strategic decisions, ranging from the further development of hazards and sustainability indicators, to making stakeholder concerns actionable in R&D and standardisation processes.

Ultimately, while aiming to remain explicitly sensitive to plurality in terms of valuing "good chemicals", the contribution places the emphasis on how this kind of anticipatory work can help to surface tensions early and to keep options open as evidence and requirements evolve.[3] It concludes with proposals for strengthening interdisciplinary collaboration and for harmonising advances in chemicals and materials with the global need for sustainability, clarifying how the current attention to SSbD can inform more robust, forward-looking pathways for chemical innovation.

Insights for this contribution were gathered through participation in the ongoing BIO-SUSHY project, funded by the EU under the Grant Agreement no.101091464.

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RC - D1 - O07
The death of chemophobia - Revisiting the public image of chemistry

Christian Schnurr[1]
[1]*Environmental Science Center, University of Augsburg, Germany; Chair of Analytical Food Chemistry, Technical University of Munich, Germany*

The talk engages from a historical and philosophical perspective with the concept of ‘chemophobia’, which strongly shapes debates about the public image of chemistry. The concept was initially popularized in the 1960s by US-American nutritionist Douglas Van Anden Frost, in order to criticize regulations on arsenic in foods. Since then, the concept has spread widely among communities of toxicologists, chemists, and food scientists, and has been adopted in risk and consumer studies. Currently, the marketing trend to advertise consumer products as ‘free from chemicals’ or ‘only natural’ has brought chemophobia debates back on the menu. Being inherently normative, the allegation of ‘chemophobia’ is typically brought forward by members of the chemistry community against the general public, political regulators, the media, or advertising, intending to describe an exaggerated, irrational fear of industrially-produced chemicals; a flawed risk perception, it is assumed, leads to irrational consumer choices, undermines public trust in regulatory institutions and dampens chemistry’s social status.
The talk puts forward arguments against the concept of ‘chemophobia’. First, empirical studies indicate that the public image of chemistry is significantly less negative than members of the chemistry community anticipate. Rather, assuming ‘chemophobia’ has become part of the disciplinary self-identity of chemists, a phenomenon that has itself been called ‘chemophobia-phobia’. Second, some of the arguments used ‘in defense of chemistry’ are based on similar fraudulent logic to the ‘chemophobic’ claims they attempt to counter. Third, from the perspective of public understanding of science, the chemophobia debate repeats hierarchical patterns of science communication that have been criticized as counterproductive as early as the 1980s by sociologists of science. Finally, the talk proposes alternative concepts to describe negative public sentiments towards the technoscientific products of chemistry (e.g., ‘toxicovigilance’) and suggests a rebranding of the debate on chemical risks.

RC - D1 - O08
A world without PFAS?

Rudy Dams[1], Bruno Ameduri[2]
[1]Rudy Dams Consulting, Belgium; [2]Institute Charles Gerhard, University of Montpellier, France

Per- and polyfluoroalkyl substances (PFAS) are man-made compounds involved in many industrial compositions and consumer products. Largest volume PFAS are refrigerants and fluoropolymers. Major concerns for our society related to these substances are their persistence, contribution to global warming and the potential to adverse effects on living organisms, particularly by long-chain perfluoroalkyl acid derivatives. Restrictions on manufacturing and on applications will increase in the near future. Full remediation for historical and current contaminations of air,soil and water remains problematic, especially for ultra-short PFAS. Future monitoring of PFAS-levels and their impact on ecosystems remains important. PFAS have become integrated in the lifestyle and infrastructure of our modern society and some are likely to be part of that society for years to come in essential applications by closing the fluorine-loop.

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RC - D1 - O09
Responsible use of history: Experience from the EuChemS historical landmarks awards

Brigitte Van Tiggelen[1]
[1]*Science History Institute, Philadelphia, USA - Paris, France, and Mémosciences asbl*

In 2018, the European Chemical Society awarded the first two EuChemS Historical Landmarks, and a total of 14 sites situated in different corners of Europe have since been selected.[1]
The thought for this award was triggered by the sad observation that chemistry as such was nowhere to be found during the European year of Culture in 2018 (only as a preservation of heritage technique). Latin, and even less Greek, is not anymore at the core of a common education curriculum for decades now, yet, even at the dusk of the 21st century, flocks of young students flood Rome or Athens every year, as a mean to connect to Europe's rich cultural past. In contrast, chemistry is not considered an integrant part of our shared cultural heritage.
Yet chemists and the public alike agree that chemical sciences and technology have shaped our modern world, for better and for worse. Less visible is how European chemistry has created a sense of belonging, in the course of history, even though locutions such as "European chemical community" are widely in use. Traditionally, landmarks schemes have appealed to national pride in the 19th and beginning of the 20th century. More than a place, a person or a group of persons, the EuChemS Historical Landmarks awards are therefore given to sites in Europe where events in chemistry occurred that have left an imprint in the chemical community and in our everyday world and life all together. These sites tell the stories of how chemistry developed across Europe (and sometimes beyond) through singular yet shared moments of deep transformations.
This presentation will address the important issue on how to use history in a responsible way in the present transnational tensions, keeping in line with the initial aim of the award scheme.

[1]https://www.euchems.eu/awards/euchems-historical-landmarks/

RC - D1 – O10
Discovering the elements: No simple stories

Brigitte Van Tiggelen[1], Annette Lykknes[2]
[1]Science History Institute, USA; [2]NTNU-Norwegian University of Science and Technology, Norway

In the recently published volume *Discovering the Elements. No Simple Stories* (ed. by Brigitte Van Tiggelen and Annette Lykknes, World Scientific Publishing, 2026), a collection of 9 contributions challenges the popular account of elemental discoveries which situate them as a singular moment in time and space, with clearly defined actor(s) who are deemed discoverer(s). The book also provides didactic materials to promote these discussions in the classrooms.
Based on the analysis of chosen examples and visuals from element discoveries, the editors/presenters will discuss the complexity of scientific discoveries, and the way they are narrated, in the form of a dialogue that will offer food for thought and open for a wider conversation on the topic.

RC - D1 - O11
Teaching about Crookes's *Vis Generatrix* model of the periodic system

Annette Lykknes[1]
[1]*NTNU-Norwegian University of Science and Technology, Norway*

The physicist and chemist William Crookes is remembered for his discovery of thallium, his innovate work in spectroscopy and radioactivity, his invention of the Crookes tube and the radiometer, his role as founder and editor of *Chemical News*, among other things.
In 1888/1898, Crookes introduced a three-dimensional model of the periodic system—a figure-eight shaped spiral constructed by his assistant, James H. Gardiner—which he called *Vis Generatrix*. This model sought to illustrate the "creation of the elements," drawing on the concept of primary matter, or "protyle," first proposed by William Prout in the early nineteenth century. I have explored this model in a pedagogical context, using it as an example of three-dimensional representations of the periodic system.
In 2019, a group of student teachers enrolled in a history of science course at the Norwegian University of Science and Technology (NTNU) were tasked with reconstructing Crookes's model, working from photographs, drawings, and dimensional measurements provided by the Science Museum in London. The exercise provided students with valuable learning opportunities on several levels: it served as a lesson in the history of science and nineteenth-century ideas about the creation of the elements; it offered a window into the Nature of Science (NOS); and it invited reflection on the role of models and historical perspectives in their own future practice as teachers.
In this presentation, I will report on the exercise and reflect on how learning about, and engaging with, 3D models of the periodic system such as Crookes's can contribute to the education of today's pre-service science teachers.

RC - D1 - O12

Implementation of the course “good chemistry: Methodological, ethical and social dimensions” at Jagiellonian University in Krakow (2019-2026)

Iwona Maciejowska[1]
[1]*Jagiellonian University in Krakow, Poland*

This presentation discusses the multi-stage implementation of the course Good Chemistry: Methodological, Ethical and Social Dimensions at the Faculty of Chemistry, Jagiellonian University in Krakow. Four academic years are covered: a nationwide fully online pilot (2019/202) and blended-learning editions (2023/24, 2024/25), delivered via the EuChemS Moodle platform, followed by a blended-learning edition implemented on the Jagiellonian University’s e-learning platform in 2025/26. The course concept, structure, and pedagogical design are based on content and learning activities developed primarily by Prof. Jan Mehlich and further elaborated in his book.

The course introduces students to research methodology, scientific integrity, ethical reasoning, sustainability, the social responsibility of chemists, and science communication. In the blended format worth 3 ECTS, students individually select seven out of fifteen remotely completed modules according to their interests. Across editions, the most frequently chosen modules were Scientific Method, Scientific Misconduct, and Animal Experiments. The course was completed by 25 students in both 2023/24 and 2024/25, and by 28 students in 2025/26; each cohort included six Erasmus exchange students.

The presentation analyses student engagement and evaluation data from all editions. Identified strengths include strong involvement in case-based activities and sustained reflection on students’ own research practices. Challenges included difficulties with terminology originating outside the traditional STEM curriculum and engaging with perspectives perceived as distant or controversial within scenario-based tasks.

To address limited interaction in asynchronous discussions observed in earlier editions, subsequent course iterations introduced redesigned warm-up activities, more structured discussion prompts, and onsite meetings aimed at fostering community building, trust, and open expression of views.

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RC - D1 - F01

Transforming chemistry education for the green transition: A competence-based European approach

Sanjiv Prashar[1,2,3]

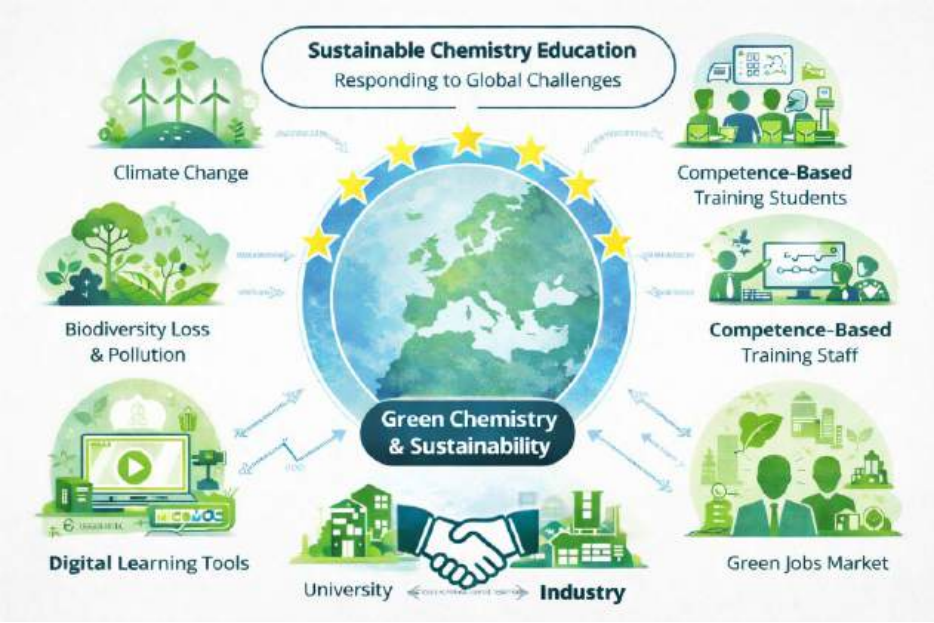
[1]Universidad Rey Juan Carlos, Spain; [2]European Chemistry Thematic Network, Belgium; [3]Instituto de Tecnologías para la Sostenibilidad, Spain

Global challenges such as climate change, resource depletion, biodiversity loss and pollution demand a profound transformation of chemistry education. Higher education institutions play a critical role in preparing future chemists with the knowledge, skills and attitudes required to contribute to the green transition. This presentation presents an educational framework developed within a European cooperation partnership, including the European Chemistry Thematic Network, aimed at integrating sustainability and green chemistry competences into university-level chemistry curricula.

The initiative focuses on the development of Green Competence Profiles aligned with European sustainability frameworks, including the European Green Deal and the GreenComp sustainability competence framework. These profiles are designed to support competence-based, interdisciplinary and research-informed learning approaches in chemistry education. Particular emphasis is placed on the systematic integration of green chemistry principles, bioeconomy concepts and life-cycle thinking into existing curricula, rather than treating sustainability as an isolated topic.

The framework combines curricular innovation with pedagogical and digital transformation. Key activities include comparative analysis of existing competence models, design and testing of sustainability-oriented competence frameworks, and development of modular teaching and training resources. Digital tools such as microMOOCs, online assessment platforms and blended learning approaches are employed to enhance accessibility, flexibility and learner engagement. In parallel, professional development activities target both academic staff and industry professionals, strengthening links between higher education and the evolving green labour market.

At the European level, the proposed approach supports convergence in sustainability teaching and contributes to shared educational standards in chemistry. Expected outcomes include enhanced teaching materials, trained educators, strengthened university–industry collaboration, increased student awareness of sustainability issues, and the establishment of a European Green Chemistry Community of Practice to ensure long-term collaboration, dissemination and policy impact.



RC - D1 - F02

Implementing sustainability competences and practices at Quy Nhon University, Vietnam

H. Mimouni[1], Xander Bell[2], Jasper Ooghe[2], Yves Ronsse[2], Els van Mechelen[2], Chi Vo Van[3], Thanh-Lieu Thi Le [3], Dang Thi To Nu[3], Vera Meynen[1]
[1]University Antwerp, Belgium; [2]HOGENT, Belgium; [3]Quy Nhon University, Vietnam

Sustainability competences are essential for current and future scientists. To adapt these practices to education, QNU chose to fully embed sustainability on Campus, from the campus wide practices down to the course content itself. In a joint effort between Quy Nhon University (QNU, Vietnam), HOGENT and UAntwerp, through a VLIR UOS project, safety and sustainability at QNU were critically evaluated and adapted both in a Campus wide approach, by e.g. adapting infrastructure and waste recycling practices on Campus, and down to sustainable use of chemicals in student chemistry laboratories.

Participative learning of students was introduced, involving them in the process of developing a more sustainable campus and educational program. Rethinking practical laboratory courses, safety and waste management were some of the initiatives. In a joint effort between Belgian and Vietnamese staff and students, the existing chemistry laboratory courses were critically evaluated.

After introductory safety and sustainability courses (including e.g. lectures and video's), the students developed a simple risk-analysis tool with objective green metrics to score the reagents, solvents, additives, mixtures and products formed in the experiments towards safety and environmental impact. The aim of the scoring was to substitute the worst scoring educational practicals with safer and more environmental benign alternatives, without sacrificing the educational didactic goal of the practical. If substitution was not possible, greener alternatives were looked for. In a first step, the general chemistry laboratory was evaluated, resulting in 8 out of 11 experiments where a safer and/or environmentally more friendly substitution/alternative was found. Moreover, also a waste management plan was set up. Next, the methodology was introduced into the educational package to provide the students with metrics based safety and environmental assessment competences applied to their laboratory courses.

This way normative, strategic and awareness competences were introduced in sustainable education as well as interpersonal and intercultural competences valuing cooperation and joint learning from interregional collaboration[1,2].

This research is being conducted within the framework of IUC-QNU. We acknowledge the support of VLIR UOS for funding the Institutional University Cooperation (IUC) - QNU Program phase 1 under the program code VN2022IUC044A101. This work is part of the SP7 subproject: "Establishment of a sustainable lab management system and an institutional waste management system (IWMS) at QNU"

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RC - D1 - F03

The ECTN eurolecturer academy: A European platform for teaching Innovation and professional development in chemistry higher education

Iwona Maciejowska[1], Natasa Brouwer[2]
[1]Faculty of Chemistry, Jagiellonian University, Poland; [2]University of Amsterdam, The Netherlands

The European Chemistry Thematic Network (ECTN) brings together more than 100 universities from 30 countries. It has a long tradition of supporting innovation and quality enhancement in chemistry higher education. ECTN has developed a framework for the bachelor, master and doctorate qualifications in chemistry (the Eurolabel®).

Within the ECTN, the Eurolecturer Academy1 has been established as a European platform that promotes recognition of university teaching quality and continuous professional development (CPD) in chemistry and, more broadly, STEM higher education. The CPD activities for lecturers and programme directors focus on powerful, inclusive active learning approaches to teaching, learning and assessment and include online webinars, thematic workshops and intensive summer schools on teaching and learning and STEM-CPD. The STEM-CPD Summer School prepares its participants to foster CPD activities at their respective institutions and, this way, as CPD Ambassadors, successfully realize teaching innovations that are relevant for their university. The first STEM-CPD Summer School took place in 2021. At this moment, 69 CPD Ambassadors are already active and successful.2

The STEM-CPD Summer School 2026 will take place in Madrid and will focus on Union of Skills, the Erasmus+ strategy for education in Europe. A growing community of practice will improve the quality of teaching at collaborative universities and the quality of higher Chemistry education.

Our contribution will outline main activities of the ECTN Eurolecturer Academy (https://ectn.eu/work-groups/eurolecturer-academy/), share good practice, and invite participants to join the community to shape a European CPD culture for excellent and innovative university Chemistry and STEM education.

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[2]Brouwer, N., Niemelä, M., Maciejowska, I., Grecea, Ş., Tarallo, O., & Russo, V. *Chemistry Teacher International* **2024**, 6, 201-216.

RC - D1 - F04

Educating future chemists for sustainable transformation: Digital and competency-based approaches across vocational and higher STEM education

Silke Fähnemann[1], Aglaia Angolini[1], Jann Schneider[1], Dana Sommerfeld[2], Matthias Hirschmann[2], Arne Cierjacks[1], Kathrin Harre[1]

[1]Hochschule für Technik und Wirtschaft Dresden, Germany; [2]Ausbildungsverbund Olefinpartner gGmbH, Germany

Equipping future chemists and STEM professionals with sustainability and green chemistry competencies is a key prerequisite for advancing the transition toward climate-neutral, resource-efficient, and socially responsible chemical systems. This contribution presents two complementary educational formats that translate sustainability principles into future-oriented learning designs, combining digital instruction, competency-based education, and transformative project work across vocational and higher education.

Within the MONAMINT project, a modular digital course has been developed to introduce vocational STEM learners to fundamental concepts of sustainable development, green and resource-efficient chemistry, and environmentally responsible technological practices. The course is designed for flexible integration into diverse vocational training pathways and provides a scalable framework for systematically embedding sustainability competencies into existing curricula. Digital learning units are complemented by interactive workshops that empower trainers and industry partners to integrate sustainability perspectives into everyday training and professional practice.

At HTW Dresden, a sustainability module has been established within a newly introduced sustainability certificate program. By integrating online foundational learning with intensive block seminars, the module promotes inquiry-driven and project-based learning. Through the development of individual sustainability projects, particularly addressing contributions to the ecological handprint, students are encouraged to critically reflect on the role of chemistry in shaping sustainable futures and to develop actionable solutions.

Together, these initiatives illustrate transferable pathways for embedding sustainability and green chemistry competencies across educational levels. They highlight how digital learning environments and transformative pedagogies can support the development of future-ready chemists capable of actively contributing to the European Green Deal and the broader transformation of chemical education and practice. In this way, the presented approaches directly contribute to SDG 4 (Quality Education) and SDG 12 (Responsible Consumption and Production), fostering long-term impact at the interface of education, chemistry, and sustainability.

RC - D1 - F05
Sustainability hackathon: Bridging the gap between higher education and society

Dorien Baeten[1], Ilse Engelen[1,2,3], Sarah Doumen[1], An Hardy[1,4], Wouter Schroeyers[3,5]
[1]Faculty of Sciences, Hasselt University, Belgium; [2]School of Educational Studies, Hasselt University, Belgium; [3]Faculty of Engineering Technology, Hasselt University, Belgium; [4]Institute for Materials Research, Hasselt University, Belgium; [5]Centre for Environmental Sciences, Research group NuTeC, Hasselt University, Belgium

In the transition towards a circular economy, chemists and engineers are no longer just technical experts; they are the architects of sustainable value chains. Equipping students with the necessary sustainability competencies to navigate these responsibilities is essential. Yet, traditional curricula often struggle to translate abstract sustainability goals into practical, professional skills. This contribution highlights how the 'Sustainability Day', an interdisciplinary hackathon organized at UHasselt, bridges this gap by transforming theory into hands-on, responsible innovations.
This Sustainability hackathon is a key output of an ongoing VLAIO-funded project that aims to embed the Sustainable Development Goals (SDGs) into educational programs. The project focuses on building a structural 'Sustainability' learning line within the programs of Industrial Engineering (KU Leuven/UHasselt), Chemistry, Physics, and Materiomics (UHasselt). By making implicit sustainability elements explicit and integrated, we increase their visibility and foster a systematic development of our students' professional identity as responsible societal actors.
The 'Sustainability Day' is a practice-oriented learning initiative that makes sustainability competencies tangible. Structured as an intensive hackathon in collaboration with industrial partners and Vlajo, the event challenges master students to analyze actual sustainability cases and develop feasible solutions within interdisciplinary teams, hereby simulating a professional R&D environment. Teams are guided by expert coaches from both industry and academia, ensuring that solutions are grounded in current professional expectations. The trajectory encompasses the entire innovation cycle: from deep-dive problem analysis and collaborative brainstorming to a final pitch for a professional jury. This authentic learning context stimulates students to bridge theory with skills such as systems thinking, critical analysis, creative problem-solving, and effective communication.
This contribution presents a practical approach for educators to move beyond theoretical SDG instruction. By sharing our experience with this model, we provide insights into how high-impact learning environments can effectively bridge the gap between higher education and society.

RC – D1 - F06
Green infrastructure and built heritage in historic cities under climate change

E. Zendri[1], S.M. Preo[1], A. Orler[1], L. Falchi[1], E. Balliana[1], F.C. Izzo[1], M. Gnemmi[1], M. Zucchelli[1], A. Cairoli[1,2], G. Buffa[1], E. Fantinato[1]
[1]Dept. of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Italy; [2]Dept. of Classics, Sapienza University of Rome, Italy

The increasing frequency of adverse climatic events represents a major challenge of climate change, threatening both natural and cultural assets in urban environments. Green infrastructures are widely recognised as a key climate change mitigation strategy [1]. It contributes to microclimate regulation, pollutant mitigation, and the reinforcement of cultural identity, However, it also increases risks related to moisture retention, biodeterioration, and the deposition of organic matter on built surfaces [2]. Addressing this duality requires interdisciplinary approaches grounded in material science and analytical chemistry.
The scientific understanding of the relationship between urban green areas and the conservation of cultural and architectural heritage remains fragmented, particularly from a chemical and material perspective. Within this framework, the JPI project ATLAS develops an integrated assessment system to investigate the relationship between green infrastructure and immovable cultural heritage in historic urban contexts. The assessment focuses on architectural sites located in proximity to selected urban green areas. It is based on three indices (vulnerability of cultural heritage assets in relation to green areas, anthropic pressure, and cultural and architectural value), which are described by qualitative and quantitative indicators. The framework is supported by analytical investigations aimed at characterizing material interactions at the interface between vegetation and heritage surfaces.
As part of the assessment, samples of deposits were collected from 47 surfaces across 12 historic buildings in the city of Treviso (Italy) every 2 months for a total of 12 months, using adhesive tape and a brush. Surface morphology and deposits were investigated using optical and electron microscopy, Raman and FTIR spectroscopy, and chromatographic techniques (Fig.1). Preliminary results indicate that the proximity and characteristics of green infrastructure influence surface deposition processes and deposit composition, highlighting the need for balanced management strategies considering both conservation risks and the ecological and social benefits of green infrastructure in historic urban landscapes.

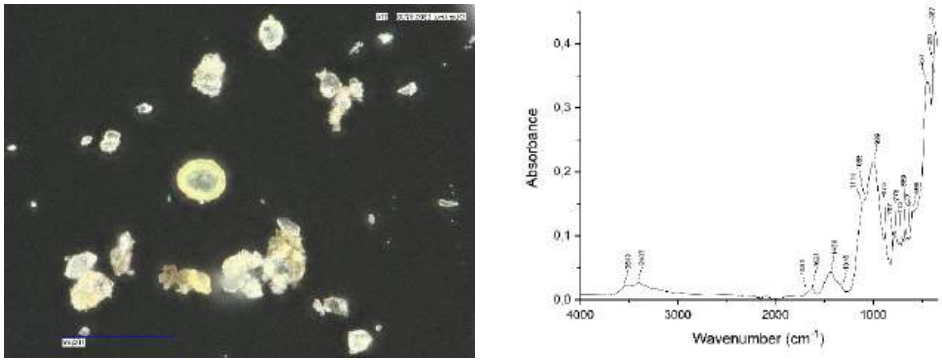

Fig. 1. Example of the morphological aspect of deposition collected from a building in Treviso (Santa Caterina Church) (left) and chemical characterization by FTIR spectroscopy (right).

Acknowledgements: This research is supported by the CH-JPI project ATLAS "Studying symbiotic scenarios linking Heritage assets and green areas to prepare Historic Cities to face Climate Changes"

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[2]Gadd, G. Geomicrobiology of the built environment. *Nat Microbiol* 2, 16275 (**2017**). https://doi.org/10.1038/nmicrobiol.2016.275

RC - D2 - O01
The best 3 seconds of my life: Igniting passion for chemistry through short-form videos

David Mareš[1], Pavlína Konopáčová[2,3], Michal Řezanka[2,3]
[1]Faculty of Mechatronics, Informatics and Interdisciplinary Studies, Technical University of Liberec, Czech Republic; [2]Faculty of Science, Humanities and Education, Technical University of Liberec, Czech Republic; [3]Department of Nanochemistry, Technical University of Liberec, Czech Republic

In today's digital landscape, it has become increasingly challenging to make chemistry and science engaging on the internet. Current trends are dominated by short-format videos, where creators must capture attention within the first three seconds or risk losing the audience entirely. This pressure fundamentally changes how scientific content is designed, communicated, and perceived by the public.
This contribution presents our experience with the Instagram account @onch_tul[1], focused on the popularization of chemistry through short, visually engaging, and often humorous videos rooted in real laboratory practice. Over a period of 15 months, the account has grown to more than 13,500 followers, with continuous organic growth, and has accumulated tens of millions of views across its content. These results demonstrate that even traditionally "difficult" topics such as chemistry can reach a broad audience when adapted to the dynamics of modern social media platforms.
The presentation will discuss content strategies, storytelling approaches, and the balance between scientific accuracy and entertainment value that proved effective in short-form formats. Special attention will be paid to the role of the opening seconds of a video, audience retention, and the use of trends without compromising scientific integrity.
Finally, future plans will be outlined, including the expansion to additional social media platforms and a systematic comparison of how chemistry and science communication perform across different digital environments. The goal is to better understand platform-specific dynamics and to further develop effective tools for inspiring public interest in chemistry and science.

[1]Department of Nanochemistry (@onch_tul). https://www.instagram.com/onch_tul/.

RC - D2 - O02

Designing immersive chemistry education: An educational game on catalytic CO_2 valorization

Thomas Hartman[1,*], Martijn Hut[1], Max Weel[2], Thomas Wind[3], Henri Matimba[4], Wouter van Joolingen[4], Bert Weckhuysen[1]

[1]Institute for Sustainable and Circular Chemistry, Dept. of Chemistry, Utrecht University, The Netherlands; [2]Raccoon Serious Games (dissolved), The Netherlands; [3]Educate-it, Utrecht University, The Netherlands; [4]Freudenthal Institute, Utrecht University, The Netherlands

We have developed and implemented an educational game designed to enhance learning (experience) for Bachelor's students in the Catalysis course at Utrecht University and to train the next generation of chemists to think critically and analytically. By connecting theory and real-world context we prepare them to tackle multi-disciplinary societal problems, like climate change and sustainability challenges. Game-based learning can support in this mission as they can effectively enhance students' conceptual understanding and critical skills.[1] By applying Design Thinking principles, we created a first-person simulator that immerses students as researchers on a spaceship. Their goal is to solve a water crisis by researching and optimizing the Sabatier reaction (CO_2 + 4 H_2 → CH_4 + 2 H_2O). In the digital world, we give students the freedom to study, experiment, and rehearse core catalysis concepts with direct feedback using simulated reactions and analytical tools, while working at their own pace (Figure 1). Additionally, the game mechanics are intrinsically integrated with the course content to further enhance intrinsic motivation.[2,3] Besides learning the catalysis course content, students also improve their understanding of research and analytical sciences.

We evaluated the game using a mixed-methods approach, including anonymous surveys, anonymized focus group interviews, and analysis of screen capture videos. The students praised the game's accessibility, engagement and educational value and were immersed in the game and felt motivated by the game mechanics to continue learning and experimenting. The analysis of the results furthermore gave insights to improve future modules and expansions.

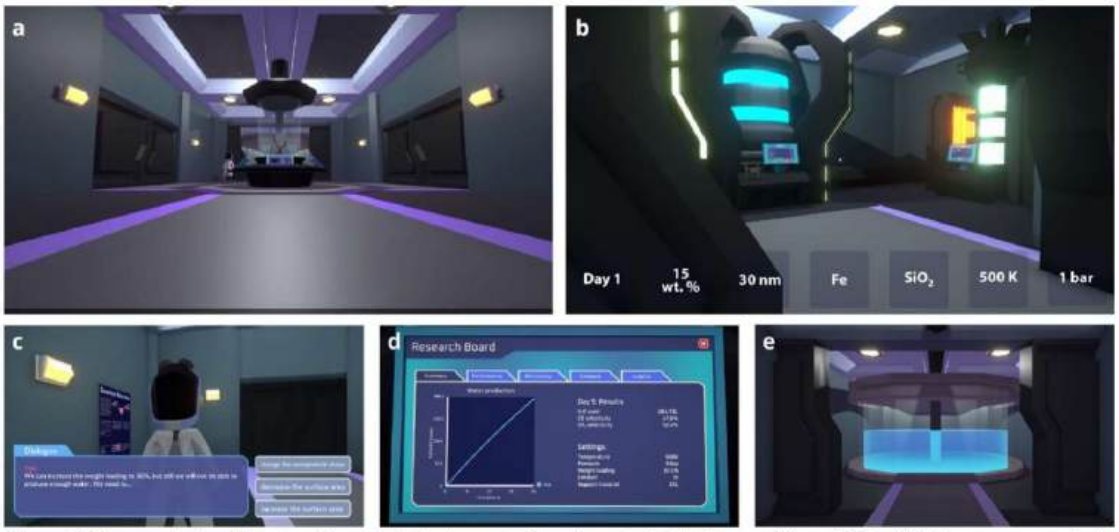

Figure 1. Screenshots of the developed catalysis game focusing on the hydrogenation of CO_2 with H_2 over supported metal catalysts. The students can walk through the **(a)** spaceship and interact with **(b)** equipment to perform various experiments, discuss their findings with **(c)** a non-playable Research Assistant, analyze their results using the **(d)** Research Board to find the optimal catalyst and conditions for the production of **(e)** water to save the crew.

Acknowledgements: This work was funded by the fUSO (Utrecht Education Incentive Fund). The authors would like to thank Softwareproject Informatica (Tamara Mtsentlintze and Team Buitenbeentjes) for programming the game for use as a web application, Alexander Sterk (Racoon Serious Games) for the final corrections to the playable game.

[1]Hu, Y.; Gallagher, T.; Wouters, P.; van der Schaaf, M.; Kester, L. *J. Res. Sci. Teach.* **2022**, *59*, 1499-1543.
[2]Habgood, M. P. J.; Ainsworth, S. E. *J. Learn. Sci.* **2011**, *20*, 169-206.
[3]van der Linden, A.; Meulenbroeks, R. F. G.; van Joolingen, W. R. *J. Comput. Assist. Learn.* **2024**, *40*, 1500-1510.

RC - D2 - O03
Smarter chemistry teaching with artificial intelligence

Luis Bello[1]
[1]*Tulsa Community College, USA*

This presentation shares practical insights into the integration of artificial intelligence (AI) tools in teaching General Chemistry at Tulsa Community College, Oklahoma. Based on classroom experience, it demonstrates how AI technologies have significantly improved both student engagement and instructional effectiveness.
One major application has been the use of AI-driven platforms to deliver personalized, timely feedback on digitally submitted lab reports. This not only accelerates the grading process but also ensures students receive actionable feedback more quickly enhancing their learning outcomes and academic performance.
A further innovation includes the real-time creation of interactive classroom activities using tools like Google Gemini, ChatGPT. These platforms enable spontaneous generation of quizzes, in-class exercises, and formative assessments, all without the need for prior preparation or physical materials—fostering a flexible and paperless teaching environment.
AI-assisted digital notebooks have also been utilized to develop video content and multimedia study resources that align with laboratory procedures and course topics. These tools support visual and auditory learning styles, helping to make complex concepts more accessible and engaging for all students.
Moreover, AI has played a crucial role in analyzing student performance data. For example, it revealed consistently low achievement in a thermodynamics lab activity, prompting a redesign of the lab and the creation of targeted instructional supports. This data-informed intervention led to measurable improvements in student understanding and success.
Overall, the use of AI in the chemistry classroom has gone beyond automation. It has empowered more adaptive teaching strategies and a learner-centered approach—paving the way for a more responsive, efficient, and inclusive educational experience.
Integrating AI tools into General Chemistry instruction has enhanced feedback, engagement, and learning outcomes. By streamlining assessment, supporting multimedia resources, and enabling data-driven interventions, AI empowers educators to create a more dynamic, responsive, and effective educational environment for today's diverse student population.

[1]Bello, L (2025). Enseñar con Inteligencia Artificial: Guía Práctica desde el Aula: Redefiniendo la Educación con IA: Conceptos y Casos Prácticos (Spanish Edition) Paperback – May 22, **2025** https://a.co/d/gaHkIHQ
[2]Bello, L. ; Aubert L. (2024) AI in the Classroom: Democratizing Knowledge and Transforming Education. DOI: https://doi.org/10.22533/at.ed.385132504049
[3]Bello, L. (2023). La inteligencia artificial (IA) como catalizador de la transformación educativa. Editora Artemis. Retrieved April 4, **2025**, from https://editoraartemis.com.br/catalogo/post/la-inteligencia-artificial-ia-como-catalizador-de-la-transformacion-educativa
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RC - D2 - O04

European chemistry thematic network core chemistry 2026: A renewed framework for first-cycle chemistry education in Europe

Sanjiv Prashar[1,2]
[1]Universidad Rey Juan Carlos, Spain; [2]European Chemistry Thematic Network, Belgium

The European Chemistry Thematic Network (ECTN)[1] has updated its Core Chemistry recommendations for bachelor-level chemistry programmes, more than 20 years after the first list of core topics linked to the Bologna Process.[2] This contribution presents the structure, content, and intended use of the new Core Chemistry brochure and its role in strengthening quality and convergence in European chemistry education.

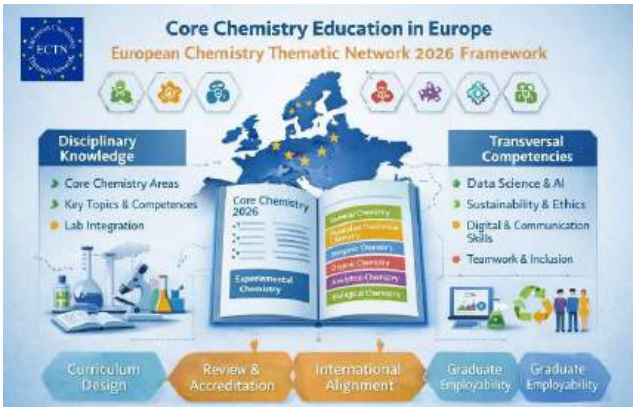
Core content is defined as material taught in at least 80% of European bachelor programmes in chemistry. The brochure structures recommended content and learning outcomes across six domains: General Chemistry, Physical and Theoretical Chemistry, Inorganic Chemistry, Organic Chemistry, Analytical Chemistry and Biological Chemistry, with a separate chapter on Experimental Chemistry. For each area, the document specifies key topics, explanatory details, and explicit competences / learning outcomes, with strong emphasis on systematic integration of laboratory practice with theory.

Beyond disciplinary knowledge, transversal competencies are emphasised. These include research data management and data science (including electronic laboratory notebooks and national research data infrastructures), sustainability and ethics (UN SDGs, Green Chemistry, Hague Ethical Guidelines), digital competence and responsible use of artificial intelligence, communication and presentation skills, teamwork, diversity and inclusion, and an understanding of chemistry as a global enterprise.

he document is conceived as a flexible reference rather than rigid requirements. It is intended to support curriculum design, review, accreditation, and alignment with ECTN Eurolabels® and EChemTest®, while allowing adaptation to national regulations and institutional strengths (e.g. materials science or specialised tracks).

The presentation outlines the revision process and stakeholder involvement, highlights the main innovations compared to earlier recommendations, and discusses how the new framework can be implemented to enhance graduate employability and to ensure that bachelor graduates acquire robust disciplinary foundations together with digital, sustainability-related, and generic skills.

Thanks to all those involved in the ECTN Core Chemistry working group.[3]



[1]https://ectn.eu/
[2]https://tuningacademy.org/wp-content/uploads/2014/02/RefChemistry_EU_EN.pdf
[3]https://ectn.eu/work-groups/the-core-chemistry/

RC - D2 - O05
Simple(r), yet (more) efficient maths teaching for students of chemistry

Dirk Andrae[1]
[1]*Freie Universität Berlin, Germany*

More than 180 years ago, Justus Liebig, known today as one of the founders of organic chemistry, clearly stated that "in many respects chemistry is analogous to mathematics".[1] Yet, until today, many students of chemistry struggle with huge problems in mathematics. I will show, with examples, that skills which are very helpful for chemistry studies, e.g., strength in pattern recognition (identifying functional groups in structural formulas of an organic compound), can significantly help in acquiring mastery in mathematics as well, especially if combined with efforts "to make things as simple as possible, but not simpler". All efforts, however, will not really help to remedy mathematical illiteracy among students of chemistry unless further stumbling blocks, which will be addressed, are removed.

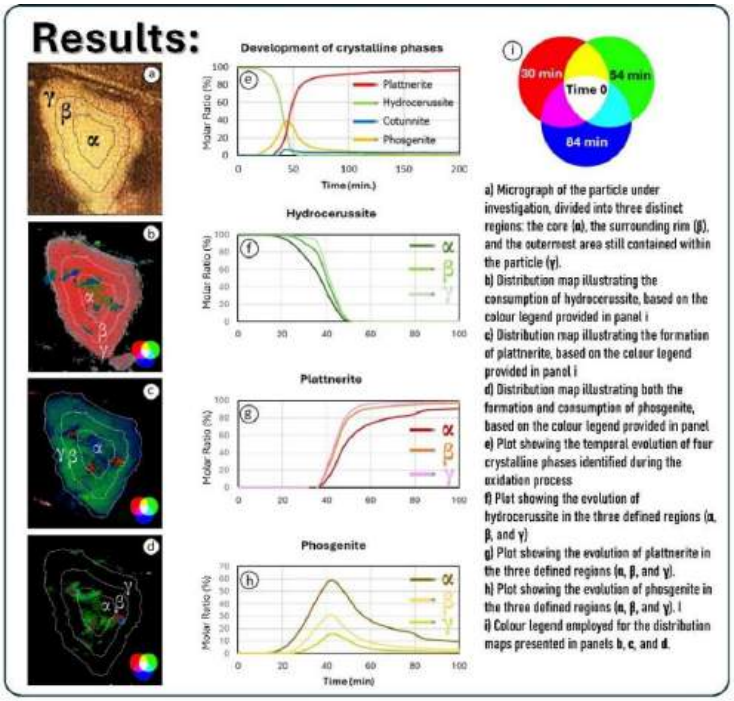
[1]Liebig, J. *Familiar Letters on Chemistry*; Taylor & Walton, 1844, p. 11 (Letter I).

RC - D2 - O06
In-operando investigations of pigment degradation processes

Ermanno Avranovich Clerici[1], Frederique Broers[2], Ramon Oord[3], Andrea Marchetti[4], Gert Nuyts[1], Letizia Monico[5-6], Katrien Keune[2], Florian Meirer[3] and Koen Janssens[1-2]
[1]AXIS Research group, NANOlab Center of Excellence, Belgium; [2]Rijksmuseum, The Netherlands; [3]ARC CBBC, Utrecht University, The Netherland; [4] ARCHES, University of Antwerp, Belgium; [5]SMAArt Centre, University of Perugia, Italy; [6]CNR-SCITEC, Italy

Effective conservation and preservation of valuable art objects such as oil paintings is based on the knowledge of the spontaneous chemical reactions that influence the constitutive materials under examination and of their kinetics. In-depth knowledge of the parameters of secondary product formation in cultural heritage materials is highly relevant for predicting deterioration phenomena and for mitigating them. Inspired by the kinetic investigations already performed during *in-operando* studies of catalysts and battery cells, a similar approach was implemented for the study of the transformation of reactive paint systems. For this purpose, a series of time-resolved experiments at the P06 micro/nano probe beamline of the PETRA III synchrotron (Hamburg, DE) was performed. The goal was to explore the behaviour of inorganic pigments undergoing spontaneous chemical modification during exposure to different atmospheric conditions (sensitivity to light and/or relative humidity) or to specific polluting gas mixtures. As means of monitoring the ongoing transformations, a combination of several relevant X-ray based imaging methods were employed, such as X-ray absorption (XAS), X-ray powder diffraction (XRPD) and ptychographic microimaging in 2D as well as 3D (tomography). In this presentation, focusing on the reactivity of crystalline lead-based pigments, only data obtained using X-ray powder diffraction imaging will be shown. As a follow up of the studies performed by Avranovich et al.[1] and Kotulanová et al.[2], a combination of synchrotron and lab-based observations at the University of Antwerp were used to model and define in detail how Pb^{4+} species are formed from lead carbonates under the influence of oxidizing agents. Specifically, the effect and involvement of HOCl in the transformation of lead white (mainly hydrocerussite – $2PbCO_3.Pb(OH)_2$) into phosgenite ($PbCO_3.PbCl_2$) and onwards into plattnerite (β-PbO_2) was explored, as plotted in Figure 1.

We acknowledge DESY (Hamburg, Germany), a member of the Helmholtz Association HGF, for the provision of experimental facilities. Parts of this research were carried out at PETRA III. Data was collected using the micrometer diffraction beamline P06 provided by DESY Photon Science. We would like to thank Gerald Falkenber, Ken Vidar Falch, and Dennis Brückner for assistance during the experiments. Beamtime was allocated for proposals: BAG-20230002 EC



[1]Avranovich E. et al.; *Molecules* **2023,** 6106.
[2]Kotulanová E. et al.: *J. Cul. Her.* **2009**, 367-378.

RC - D2 - O07
Coupling the chemical and mechanical properties of aged lead white oil paints

Sander van Lith[1], Sonia Bujok[4], Lukasz Bratasz[4], Katrien Keune[1,3], Joen Hermans[1,2,3]
[1]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands; [2]Conservation & Restoration, Amsterdam School of Heritage, Memory and Material Culture, University of Amsterdam, The Netherlands; [3]Conservation & Science, The Rijksmuseum, The Netherlands; [4]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Poland

An oil paint undergoes chemical changes and is exposed to changing environmental conditions in its lifetime. This combination of factors makes historical oil paints vulnerable to experience critical mechanical stresses and increases the chances of crack formation and paint loss.
In this talk, we focus on linking the mechanical properties of aging lead white (LW) linseed oil-based paints to their changing chemical composition. LW paints are highly relevant, since those paints tend to develop cracks in Old Masters' paintings. The driving forces behind crack development are still unresolved. There are many chemical processes that can alter a paint's response to stress and the sensitivity to environmental conditions. For example, continued hydrolysis and oxidation of the oil polymer network results in a loss of long-range molecular connections that can dissipate stresses, resulting in a loss of fracture toughness. On the other hand, ionomeric metal carboxylates formed during aging can act as ionic crosslinker which enhances connectivity and subsequently increases mechanical strength.
As a first step forward, we investigated the link between chemical changes and tensile properties by collecting a large ATR-FTIR spectroscopy dataset and a smaller subset of tensile tests on artificially aged LW paints. Links between the two datasets were explored using multivariate exploratory analysis and regression. Finally, we compared the chemo-mechanical relationships of our dataset with naturally aged LW oil paints (> 30 years) with a similar composition. This served as external confirmation whether mechanical change can be attributed solely to chemical change, or whether other structural factors need to be considered.

RC - D2 - O08

From photodegradation to crystallization: Imaging-based evidences of organic-inorganic degradation interaction in historical paints

Teresa Scovacricchi[1, 2], Alba Alvarez-Martin[3, 1], Arthur Gestel[1], Freederik Vanmeert[3, 1], Bertrand Thomas[2], Vaclav Krupicka[2], Jorien Duivenvoorden[4], Joen Hermans[4, 5], Caroline Tokarski[2], Koen Janssens[1]

[1]AXIS Research group, NANOlab Center of Excellence, University of Antwerp, Belgium; [2]University of Bordeaux, CNRS, Bordeaux Proteome, France; [3]Conservation and Science, Rijksmuseum Amsterdam, The Netherland; [4]Conservation and Restoration of Cultural Heritage, University of Amsterdam, The Netherlands; [5]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands

Organic lake pigments are historically significant hybrid materials formed by coordinating dyes to metal substrates. Their vivid colors played a decisive role in the visual language of Expressionism, including paintings by Van Gogh and contemporaries, yet their inherent chemical fragility has led to widespread degradation and loss of cultural value. Understanding the long-term behavior of these materials therefore represents not only a scientific challenge, but also a matter of responsible cultural heritage stewardship. This study addresses the photodegradation of geranium lake pigments, based on the brominated xanthene dye eosin, in oil-based paint systems containing lead white, one of the most widely used historical pigments. To balance scientific rigor with historical relevance, paint mock-ups were prepared to reproduce historical formulations while maintaining full control over material composition and aging.[1] This strategy aligns with principles of Responsible Research and Innovation, enabling mechanistic insight while minimizing intervention on original artworks.

An integrated, imaging-based analytical approach combining high-resolution matrix-assisted laser-desorption/ionization mass-spectrometry-imaging (HR-MALDI-MSI), infrared spectroscopy (IR), and synchrotron-radiation X-ray powder-micro-diffraction (SR-μ-XRPD) was employed. The complementary spatial information provided by these techniques reveals heterogeneous degradation processes inaccessible through bulk or single-technique analyses. MALDI-MSI visualizes stepwise debromination of eosin derivatives upon photoaging, while infrared traces molecular transformations within the organic matrix. Crucially, SR-μ-XRPD identifies a previously unrecognized Pb-Br crystalline phase ($NH_4Pb_2Br_5$), confined to the light-exposed surface of the paint layer. The findings provide the first spatially resolved evidence of a coupled degradation pathway linking organic lake pigments and lead compounds, demonstrating how interactions between coexisting materials govern long-term stability. Beyond advancing chemical understanding, this work underscores the importance of cross-disciplinary, non-destructive, and imaging-driven strategies in heritage science, offering broader evidence for research in complex, real-world systems.

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RC - D2 - O09

Entwining through history & cultural heritage: The chemistry behind iron gall inks

Natércia Teixeira[1*], Rafael Hidalgo[2], João Avó[3], Maurizio Licchelli[4], Paula Nabais[5], Vanessa Otero[5], Matteo Ferretti[4], Victor de Freitas[1], Fernando Pina[3], Maria J. Melo[5]

[1]LAQV-REQUIMTE, Faculty of Sciences, University of Porto, Portugal; [2]Facultad de Filosofía y Letras, University of Cordoba, Spain; [3]LAQV-REQUIMTE and Dept. of Chemistry, Nova School of Science and Technology, Portugal; [4]Dept. of Chemistry, University of Pavia, Italy; [5]LAQV-REQUIMTE and DCR, Nova School of Science and Technology, Portugal

A significant part of our cultural heritage was written with iron gall inks, many of which are now at risk due to ink induced corrosion. Limited knowledge of their chemical composition hinders the development of effective preservation strategies.

Following our research group methodologies1, antient ink recipes were chosen and accurately reproduced. Selected Iberian written sources, and 13thc. Andalusian technical treatise by Muhammad ibn Idrīs ibn al Qalalūsī (1210–1308) were chosen2, 3.

A multi-analytical approach was used for characterization: 1) HPLC-DAD/ESI-MS; 2) Colorimetry; 3) Raman&Infrared spectroscopies analysis. Overall, polyphenolic concentration depends strongly on the extraction method and ink recipe, and gallotannins represent 79 to 50% of all phenolic compounds3, 4.

UV-VIS-NIR and stopped-flow spectrometry and electrochemical studies allowed to understand that the crucial factor to prevent ink degradation lies in a particular Fe/polyphenol ratio 5. Kinetics explains the use of iron sulfate (FeSO4) in all ancient recipes.

Degradations studies were performed and two degradation products were identified: FeSO4 and an iron-ellagic acid complex6. Using a novel green approach based on a chemically crosslinked gel, three inks from a 6-year-old application on filter paper were selected to be cleaned. Several tests were performed, and while FeSO4 was removed within 15s of application, the iron-ellagic acid complex turned out to be more demanding.

This research revealed important knowledge that can lead to practical solutions for the conservation of historical documents and artworks.

Funding: PT national funds (FCT/MECI) through the project UID/50006/2025 -LAQV-REQUIMTE.

Acknowlegments: 2023.06024.CEECIND/CP2842/CT0010, CEECIND/01344/2021 and 2021.01344.CEECIND/CP1657/CT0028.

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[2]Rafael Hidalgo, et al. *Heritage Science* **2018**, 6 (1), 63.
[3]Rafael Hidalgo, et al., *Heritage Science* **2023**, 11 (1), 7.
[4]Natércia Teixeira, et al., *Scientific Reports* **2021**, 11 (1), 8811.
[5]Natércia Teixeira, et al., *ChemPhysChem* **2024**, e202400859.
[6]Natércia Teixeira, et al., *Heritage* **2025**, 8 (7), 261.

RC - D2 - O10

A methodology for the identification and classification of weighted silk in museum collections using Portable X-Ray Fluorescence spectroscopy (PXRF)

Alina Krotova[1,2], Chiara Vettorazzo[1,2], Jenny Moreels[1], Yvan Darcis[1], Natalia Ortega Saez[1], Koen Janssens[1,2], Geert Van der Snickt[1,2]

[1]ARCHES Research Group, University of Antwerp, Belgium; [2]AXIS Research Group, University of Antwerp, Belgium

In the 19th century in Europe and North America, silks were often treated with inorganic salts, a practice that is commonly referred to as “weighting”. Even though these fabrics are among the most rapidly degrading textiles, their presence in heritage collections remains unclear. A non-invasive technique, allowing a swift identification and classification of weighted silks, is therefore essential for monitoring. So far, the fragility and multilayered structure of garments have prevented this, as the objects often cannot be placed in the vertical position for analysis, nor can superimposed foils of fabric be measured selectively.

In this research, an approach for elemental analysis using handheld X-ray fluorescence spectroscopy (PXRF) in combination with a Zr beam stop and a plastic filter is proposed that can be employed in a depot setting. This setup was tested on standard reference materials, and mock-up fabrics representative of the six prevalent historical weighting methods and validated on historical objects. Obtained results show that the methodology can not only be used to trace weighted silk, but also to identify various sub-types, which is assumed to affect the conservation state of the textile.

This approach can help museum specialists to tailor their decision-making strategy by identifying objects that need to be prioritised for preservation treatments and understand the relative presence of weighted textiles.

This research was conducted as part of the SAFESILK Project, funded by the Research Foundation Flanders (FWO) [G060422N] and the Slovenian Research and Innovation Agency (ARIS) [N1-250].

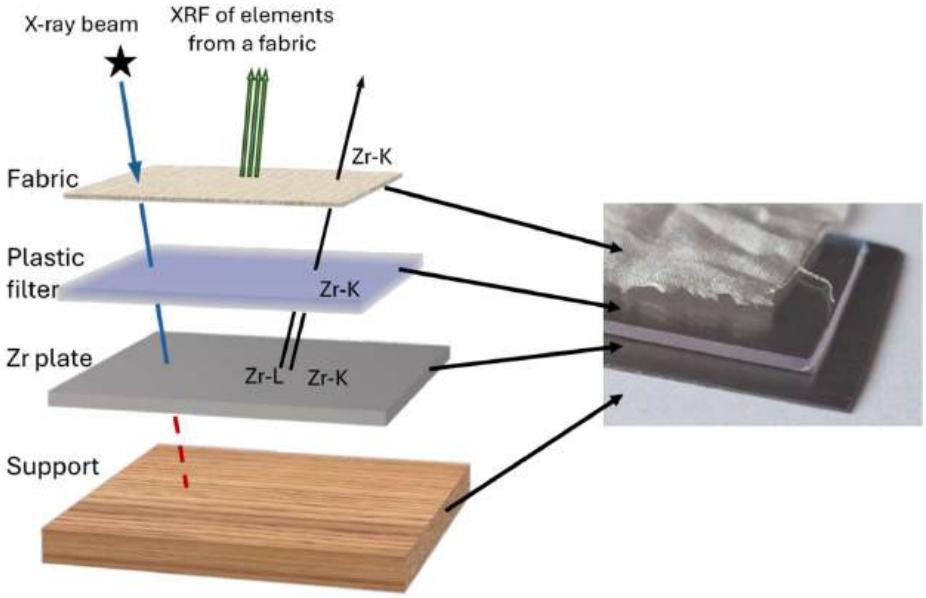


Fig. 1. A scheme illustrating the proposed setup in which a beam stop is used to enhance selectivity by absorbing the secondary radiation emitted by textile underlayers and support (tabletop or storage box), while a plastic filter blocks the low energy signals from the beam stop (Zr-L) that potentially overlap with characteristic emission lines from the weighting salts.

RC - D2 - O11

Prototype multimodal robotic system for the analysis of large-scale objects in cultural heritage, forensic science, and material inspection

Marek Kotrly[1], Josef Uher[2], Jana Bohacova[2], Ivana Turkova[1], Petr Cejka[1]
[1]Institute of Criminalistics, Czech Republic; [2]Radalytica a.s., Czech Republic

In collaboration with the Institute of Criminalistics and Radalytica a.s., a prototype multimodal robotic system has been developed for non-destructive analysis of large-scale objects in the fields of cultural heritage, forensic science, and material inspection. The system enables multispectral imaging ranging from the UV spectrum to visible and infrared light, X-ray imaging (transmission, 2D, 3D imaging, and full CT), X-ray fluorescence (XRF), and polychromatic X-ray diffraction (XRD).

The system consists of two industrial six-axis robots and is equipped with precise geometric calibration, allowing for accurate and flexible positioning of both robots. One robot carries an X-ray or multispectral source, while the other is fitted with X-ray or XRF detectors, or cameras for multispectral imaging. The size of the objects to be analysed is limited only by the range of the industrial robots used. The device is fully mobile, enabling deployment directly to the location of the event.

The next-generation X-ray imaging detectors provide high-quality images with spatial resolution at the micrometre level in both 2D and 3D imaging. Additionally, the system supports XRD phase mapping and XRF analysis. There are numerous ways to combine the XRF data with transmission maps and X-ray imaging data. The system is utilised for a wide range of applications, including art object analysis (paintings, sculptures, etc.), investigations of fire cases, industrial accidents and explosions, transport and aviation accidents, examinations of electrical devices, analysis of unknown objects and traces, and more. The volume of analytical data generated is often substantial, sometimes exceeding the operator's capacity. Consequently, in collaboration with Brno University of Technology, artificial intelligence (AI) methods are being implemented to assist operators in identifying anomalies, heterogeneities, and other relevant features.

Fig. 1. Analysis of a Large Historical Oil Painting on Canvas Using a Prototype Multimodal Robotic System.

RC - D2 - O12

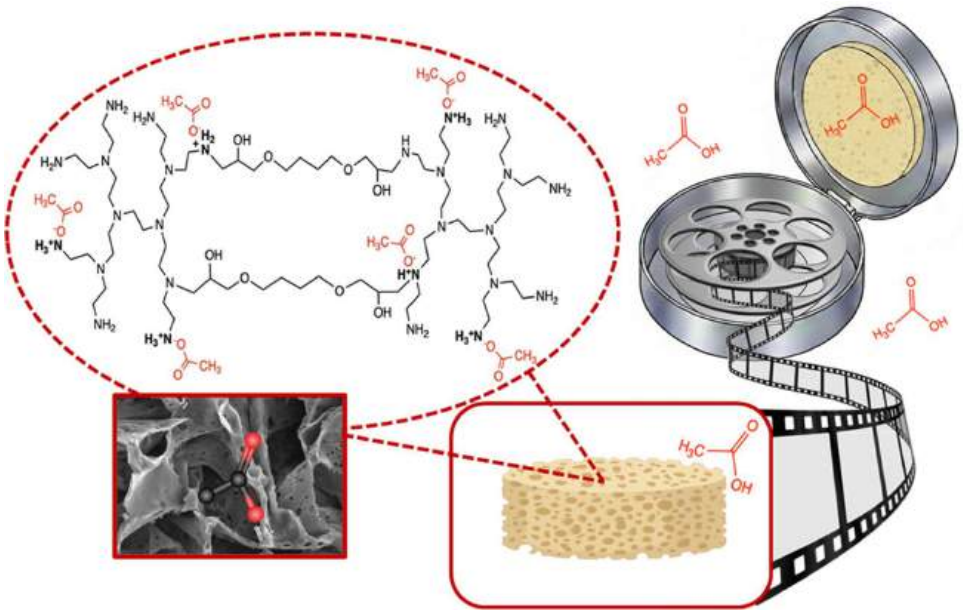
Proposal for a remediation method for the “vinegar syndrome” in cellulose acetate-based motion picture film

Francesca Porpora[1], Emiliano Carretti[1], Luigi Dei[1], M. De Sanctis[2]
[1]University of Florence and CSGI, Italy; [2]L’Immagine ritrovata SRL, Italy

Motion picture films made of cellulose acetate are subjected to chemical degradation mainly due to the “vinegar syndrome”. It concerns a deacetylation with the release of acetic acid, which acts as a catalyst for the reaction. The consequent deformation and embrittlement of the films can strictly compromise their usability[1,2]. On these bases, removing alteration by-products from the storage environment is mandatory to limit this degradation process.

The goal of this project is to set up innovative, cost-effective, user-friendly and reusable chemical inhibitors. We proposed and characterized xerogels made of polyethyleneimine (PEI)[3]. The xerogels were prepared via an epoxy–amine reaction between PEI and BDDE via cryopolymerization. This approach allows the formation of a highly porous sponge-like system, where residual free amino groups, not involved in the epoxy–amine crosslinking reaction, can neutralize acetic.

The evaluation of the efficacy of the above-mentioned systems in inhibiting the "vinegar syndrome" was performed both on real motion picture films on which the deacetylation process has been artificially induced with an innovative degradation process[4] and on films naturally affected by the “vinegar syndrome”. The different behaviors of untreated and treated films have been evaluated through an innovative multi-analytical protocol[4] able to monitor the chemical alterations of the supports connected with the occurrence and the evolution of the “vinegar syndrome”. The decrease in the acetyl content has been monitored by Fourier Transform Infrared - Attenuated Total Reflected Spectroscopy (FTIR-ATR).. In addition, the variation in mechanical and thermal properties was evaluated by Tensile Tests and Thermogravimetric Analysis (TGA).



Polyethyleneimine xerogels for the inhibition of the deacetylation process in cellulose acetate-based motion picture films.

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RC - D2 - O13
Algae for art: Sustainable bio-materials for the preservation of paper heritage

Giulia Gasperuzzo[1], Maria Grazia Ortore[2], Amina Antonacci[3]
[1]Sapienza University of Rome, Italy; [2]Marche Polytechnic University, Italy; [3]Institute of Crystallography, National Research Council, Italy

Paper-based artworks and archival documents represent a significant portion of global heritage. They are inherently prone to degradation, due to both intrinsic factors and external environmental agents Moisture accelerates the hydrolytic breakage of cellulose chains, leading to yellowing, brittleness, and loss of mechanical strength. Conservation interventions rely on organic solvents for cleaning and synthetic polymers for consolidation. However, these methods frequently present risks to human health via volatile organic compounds and carry a heavy environmental footprint.
Our aim is to develop a bio-based material that matches the efficacy of traditional products for paper conservation, while eliminating toxicity for operators. We used microalgae extracts in solution to provide a mechanical reinforcement to degraded cellulose fibres, since their bioactive properties should build a sort of protection layer against decay. Microalgae extracts' solutions are expected to have the same properties of Funori, an adhesive used for paper conservation, made from a Japanese seaweed.
These extracts were thoroughly characterized to identify the chemical composition and to measure their bioactivity, confirming significant antioxidant capacity[2]. These extracts were incapsulated in hydrogels of agarose and gellan gum. These charged hydrogels were tested on both aged and unaged paper specimens, and their efficacy was evaluated by observing variation, before and after the treatment, of the surface pH (Fig. 1), wettability and mechanical properties. AFM provided the surface characterization of the specimens at high-resolution (Fig. 2), while SANS determined any changes in cellulose structure on a nanometric scale. The results showed that our new biomaterials effectively fill the voids between cellulose microfibers, increasing surface roughness and improving structural cohesion.

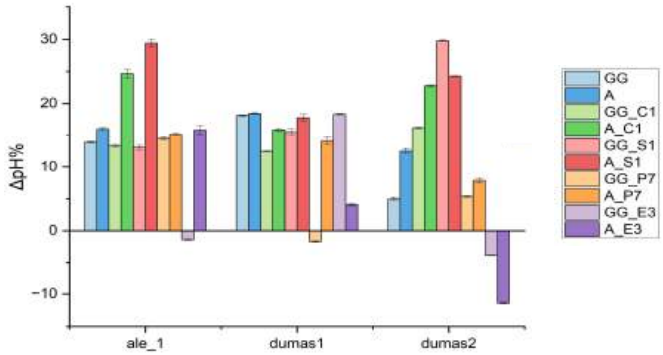

Fig. 1. variation of pH, before and after treatment

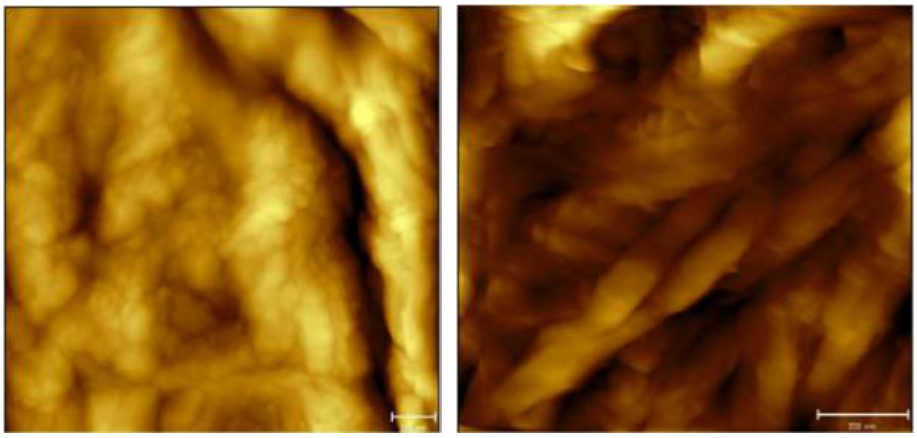

Fig. 2. AFM images of W untreated (left) and treated with Funori (right)

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RC - D2 - O14

From artifacts to batteries: Advances in muon-induced X-ray emission (MIXE) with the GIANT instrument at PSI

Xiao Zhao[1], Michael Heiss[1], Issa Briki[1], Gianluca Janka[1], Maxime Lamotto[1], Thomas Prokscha[1]
[1]PSI Center for Neutron and Muon Sciences CNM, Switzerland

Muon-Induced X-ray Emission (MIXE) is a fully non-destructive analytical technique that combines the unique properties of negative muons with the high energy resolution of high-purity Germanium detectors (HPGe) to perform depth-resolved elemental analysis. At the Swiss Muon Source (SμS) of the Paul Scherrer Institute (PSI), the Germanium Array for Non-destructive Testing (GIANT) instrument leverages a high-intensity continuous muon beam (15–60 MeV/c) to implant muons at tunable depths (μm to cm scale) in materials. The subsequent emission of muonic X-rays during atomic de-excitation provides element-specific (and often isotope-specific) fingerprints, while gamma rays from nuclear capture deliver complementary isotopic information. GIANT enables rapid data acquisition (typically <1 hour per spectrum) with exceptional sensitivity at the permille level for nearly all elements in the periodic table [1,2].
Recent applications highlight MIXE's versatility. In archaeology, the technique facilitated the confirmation of the meteoritic origin of a Late Bronze Age iron arrowhead (900–800 BCE) from Mörigen, Switzerland. The precise measurement of the high Ni (7.1–8.3 wt%) content of the bulk material further allowed to exclude the suspected local meteoritic source [3]. The analysis of a Late Antique knob bow fibula (4th–5th century CE) revealed dual bronze alloys: high-Pb cast components (12–13 wt%) and low-Pb forged parts (3.2 wt%), indicating advanced metallurgical tailoring [4]. In energy materials, MIXE paves the way for operando analyses of batteries, such as studying transition-metal plating on electrodes, which is a critical factor for improving the longevity and performance of advanced cells [5].

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[3]B. Hofmann et al*., J. Archaeol. Sci*. **2023,** 157, 105827.
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[5]F. Quérel et al., *J. Mater. Chem. A* **2025**, 13, 2275.

RC - D2 - O15
Harawayan's responsability and situated knowledges as a guide for research in chemistry

Elsje Alessandra Quadrelli[1]
[1]CNRS, Institut de Recherche sur la Catalyse et l'environnement- IRCELYON Villeurbanne, France

In the early stages of data analysis or when « values are in dispute, stakes high and decisions urgent»,[1] who we are as scientists—our values, biases, and perspectives— can shape the way we frame the research questions and how we interpret facts.[2] The accelerating pace of the Anthropocene, and the connected continuously shifting conditions of research boundaries, render these early uncertain stages probably more and more prevailing. Ignoring this human influence risks embedding hidden biases, values and perspectives into our research.[1,2,3] Integrating social science methods relevant to handle these aspects into our research toward sustainability- and in particular Organizing Research in Chemistry arund situated knowledges (see Fig)- can provide Green Chemistry with the methodological tools needed in these fast paced and uncertain times.

This presentation, argues that integrating social science frameworks -specifically Donna Haraway's concept of situated knowledge[4] which comes to term with the presence of context-based factors during the production of scientific knowledge- into Green Chemistry can be a way to produce better and more robust research outputs. By emphasizing the contextual and experiential dimensions of knowledge production, this approach aims to make Green Chemistry more accurate, inclusive, robust, just and responsive to the pressing challenges of the Anthropocene.

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[3](a) Donna Haraway "Situated Knowledges: The Science Question in Feminism and the Privilege of Partial Perspective" *Feminist Studies* **1988**, 14, 575-599. doi: 10.2307/3178066.
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RC - D2 - F01
Lipid–mineral interactions and organic residue analysis in archaeology

Yaël Antonaros[1], Francisco Mederos-Henry[2], Alicia Van Ham-Meert[3], Kristin Bartik[1]
[1]Université libre de Bruxelles, Belgium; [2]KIK-IRPA, Belgium; [3]Katholieke Universiteit Leuven, Belgium

The analysis of extracted organic residues preserved in archaeological ceramics (ORA) can provide valuable insights into ancient diets, trade networks, and ritual practices.[1] Among the recovered residues, lipid biomarkers such as triacylglycerols, fatty acids, plant sterols, and terpenoids are the most prevalent as their hydrophobic nature and chemical stability limit leaching and microbial degradation.[2]
Although lipid retention is typically linked to the porosity and bulk composition of ceramic matrices, recent studies indicate that calcite ($CaCO_3$), a common temper in archaeological ceramics, can actively influence both lipid preservation and extraction efficiency.[3,4,5] Depending on firing temperature and burial environment, archaeological ceramics may contain not only calcite but also multiple calcium phases, including portlandite ($Ca(OH)_2$), lime (CaO), and vaterite (a polymorph of calcite). Each of these phases may affect lipid preservation and retention in distinct ways, potentially introducing biases in lipid recovery and, consequently, in the archaeological interpretation of organic residues.[4,5]
Model ceramic matrices containing controlled amounts of calcite were prepared from kaolinite clay, fired and stored under different conditions. Their mineralogical composition was fully characterised before impregnation with olive oil, oleic acid, and palmitic acid. One set of samples was analysed using standard ORA protocols (grinding, extraction, GC-MS analysis) while another set was used to assess the potential of infrared imaging techniques (μFTIR and O-PTIR) for investigating lipid–mineral interactions.[6] The carbonyl absorption band serves as a key indicator for identifying lipid species within the ceramic matrix and for detecting the formation of calcium salts.
A better understanding of lipid-mineral interactions in ceramics will enhance archaeologists' ability to interpret artefact use and cultural practices with greater accuracy.

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RC - D2 - F02
Contaminated heritage: Toxic legacies in historic interiors

Natalie Daßler[1], Marianne Tauber[1]
[1]University of Bamberg, Germany

Historic monuments often conceal invisible dangers: toxic residues from past conservation and pest control practices. A newly established research group in the field of Forensic Conservation Science at the University of Bamberg investigates the interface between cultural heritage studies and analytical chemistry. The focus of an ongoing three-year research project is the detection, quantification and risk assessment of toxic heavy metals in historic interiors, ranging from rural buildings to representative castles, where pigments and conservation materials have introduced hazardous substances.
The interdisciplinary research team combines expertise in organic chemistry, archaeology, heritage conservation and the conservation of wall paintings and architectural surfaces. This allows for an integrated approach that links material characterization, environmental chemistry, and occupational health considerations. The project is motivated by the need to improve evidence-based safety standards for conservators and museum professionals who are still at risk of exposure today.
The research investigates the contamination off prestigious German castles as well as open-air museums, where materials such as wooden parquet floors, textile wall hangings, gilt leather, and feather wallpapers were historically treated with heavy metal–based pigments and preservatives. These substances, once used to protect valuable interiors, now pose significant health risks to conservators, museum staff, and visitors alike. By introducing this still underexplored field of forensic heritage science, the project addresses and highlights the ethical and practical dilemma between preserving original materials and ensuring human health and safety. By combining analytical chemistry, conservation ethics, and occupational health perspectives, the research seeks to raise awareness of the toxic legacy embedded in our cultural heritage and to encourage safer, more informed approaches to its preservation.

The authors gratefully acknowledge the Deutsche Bundesstiftung Umwelt (DBU) for funding this research project.

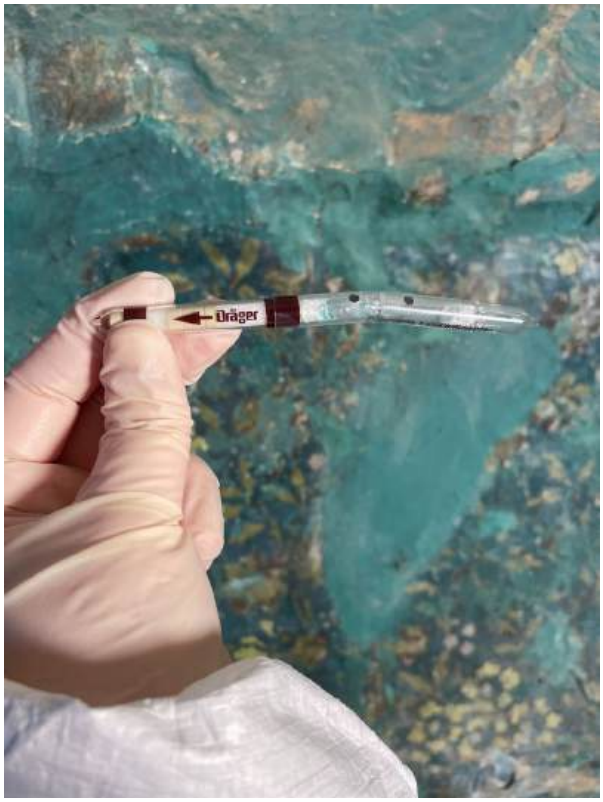

Fig. 1. Testing of colorimetric detector tubes in situ

RC - D4 - O01
AI in chemistry: Challenges, limitations, and opportunities

Michael Müller[1]
[1]*Institute of Pharmaceutical Sciences, University of Freiburg, Germany*

AI in Chemistry is seen as a prerequisite for solving major global challenges, such as the development of bioactive compounds that are less harmful to the environment and (human) health. This is a mainly technology-oriented way of thinking that may not be purposeful in the long term. Another technology-oriented concept, Green Chemistry, has been developed into a more holistic concept of Sustainable Chemistry.[1] The talk will address the question whether AI in Chemistry has the potential to develop into a lasting concept, or whether it is more a kind of 'intelligent' deflection.
Using the examples of persistent compounds, biodiversity loss, and climate change, it is shown that none of these challenges can be solved by a purely technological approach. Worse still, the hope and prospect of a (technological) solution can distract from the underlying causes and thus prevent the necessary systemic changes.[2] This results in a viscous circle: e.g., persistent compounds are released into the environment, which in turn leads to diseases that require more drugs to treat.[3] From a philosophical point of view, this leads to an unpredictability that makes evidence-based approaches even more unrealistic.[4]
In summary, we need inter- and transdisciplinary approaches in research and teaching, especially with ethics, to get closer to a concept that pursues the goal of "Sustainability". AI in Chemistry is helpful here because it is regarded the solution of last resort: if humans are intelligent, they will realize that if AI in Chemistry fails to deliver its promises as a "savior", we will have to take responsibility ourselves – the sooner (thanks to AI) the better.

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RC - D4 - O02

Chemistry for the future: On the Stockholm declaration's potential to provide practical guidance for responsible chemical research and innovation

Jan Mehlich[1]
[1]*Center for Life Ethics, University of Bonn, Germany*

Just when contemporary approaches to good professional practice in research and innovation (R&I) are challenged to be reconfigured for the tasks ahead in view of green transition policies and Green Deals, the timely Stockholm Declaration on Chemistry for the Future[1] is published and placed as a call to action for a rethinking of responsibility of chemists of all kinds. While it does not present a detailed, enforceable set of rules, it appears to be both a source of rhetorical inspiration and a foundational step toward a more concrete research integrity framework.[2] This presentation connects the visionary enthusiasm of sustainable and green chemistry as expressed in the Stockholm Declaration with the methodological and conceptual state-of-the-art of research ethics and responsible R&I. At the same time, it hopes to give due visibility to the Declaration in a way that fosters the practical changes it envisions.

The talk will examine the Declaration's content in terms of good conduct (micro-ethics) and responsible discourse (macro-ethics) approaches to chemistry for the future. It will be demonstrated that it implies the need for a personal and professional code of conduct that goes far beyond traditional research integrity since it would move from a reactive "*manage for safety*" to a proactive "*design for sustainability*" approach. This extends the chemist's responsibility beyond the lab bench to the broader economic and social systems they participate in. Ultimately, the Declaration emphasises the need for deliberative and interdisciplinary frameworks and provides the guiding principles for their development. The implementation of its vision will require further work from academic institutions, industries, and policymakers to translate its aspirational goals into concrete, actionable, and measurable practices.

[1]https://www.stockholm-declaration.org.
[2]Welton, T., et al., Stockholm Declaration on Chemistry for the Future. *RSC Sustainability* **2025**, *3*, 4187-4189.

RC - D4 - O05

Responsible AI in peptide and biomaterial design: Closing the loop from collagen-mimetic scaffolds to oxytocin analogs

Elżbieta Wojaczyńska[1]
[1]*Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland*

Artificial intelligence is increasingly used to accelerate peptide design, yet chemical workflows remain vulnerable to dataset bias, overconfident predictions, and irreproducible decision paths [1,2]. We present a responsible-AI framework implemented as a closed-loop design–synthesis–validation pipeline and demonstrate it on two complementary peptide classes. First, collagen-mimicking peptides (CMP) functionalized with rigid 2-azabicycloalkane-based analogs of proline and hydroxyproline are engineered toward thermally robust triple helices (Tm > 40 °C) and translation into hybrid hydrogel/composite scaffolds for dead-space filling under infection risk. The workflow integrates density functional theory (DFT) calculations, multi-scale molecular dynamics (including Coarse-Grained MD), and quantitative structure-property relationship (QSPR) screening combined with machine learning (ML) with experimental validation gates (CD/thermal unfolding, rheology/mechanics, degradation, and biofilm/bone marrow aspirate concentrate (BMAC) models), ensuring chemically plausible and testable outputs. Second, oxytocin analog design is used as a sensitivity stress-test, highlighting the necessity of uncertainty-aware reporting and physics-guided control layers when subtle structural changes can alter receptor selectivity and stability. We argue that responsible AI in chemistry should be evaluated not by predictive speed, but by traceability, calibrated uncertainty, and reproducible experimental outcomes.

The financial support from the National Science Centre of Poland is gratefully acknowledged (grant no. UMO-2022/47/I/ST4/02354).

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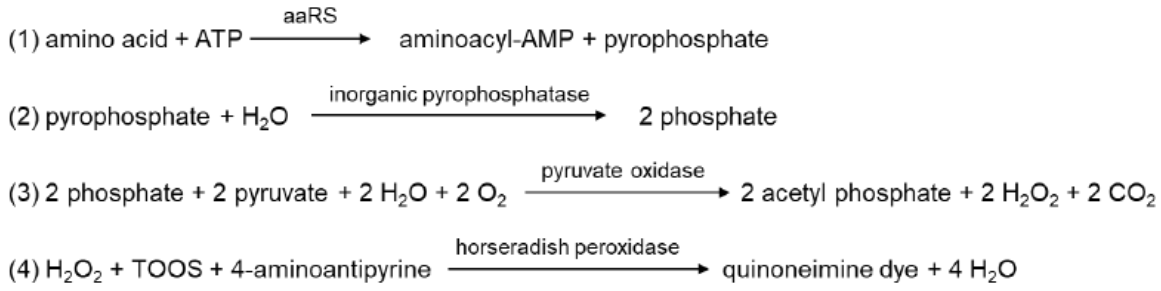
Perspectives in Analytical & Physical Chemistry (APC)

APC - D1 - P01
Development of paper-based analytical device for branched-chain amino acids

Akimitsu Kugimiya[1], Makoto Kanesada[1]
[1]Graduate School of Information Sciences, Hiroshima City University, Japan

The balances of 20 kinds of free amino acids concentration in the blood serum of healthy person are kept constant, but that of invalid person are changed in disease states, such as cancers, hepatic diseases and diabetes [1]. Therefore, the multiple disease states could be evaluated by measuring the concentrations of 20 kinds of amino acids. We have suggested the method of detecting the concentration of each amino acid using aminoacyl-tRNA synthetase (aaRS) [2, 3]. The aaRS enzyme reaction (Eq.1) and colorimetric reaction with Trinder's reagent (Eq. 4) are expressed below. These reactions were carried out on a paper-based analytical device (PAD), and the degree of color change on PAD were measured using USB camera.



In this study, a novel analytical method for the selective detection of branched-chain amino acids (valine, leucine, and isoleucine) was developed using corresponding aaRS. The responses of PADs were evaluated and from 1 to 80 mM valine, leucine, and isoleucine could be measured selectively (Fig. 1). The PADs could easily be applied to various medical checkups in the future.

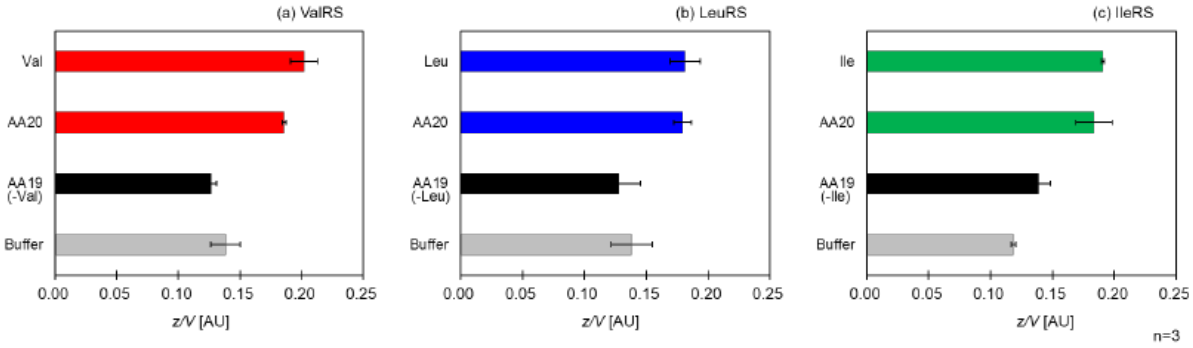


Fig. 1. Selectivity test for ValRS (a) using PADs. Substrate amino acid, 80 mM Val, a mixture containing 80 mM of 20 canonical amino acids (AA20), a 80 mM of 19 canonical amino acids excluding Val (AA19 (-Val)), and the reference buffer were applied to PADs. Similarly, (b) LeuRS and (c) IleRS.

This work was supported by JSPS KAKENHI Grant Number JP25K08827 and also supported by the Foundation Chugoku Regional Innovation Research Center.

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APC - D1 - P02

Comparative study of digestion methods for antimony analysis in certified ore reference materials

Olga Chalkiadaki[1], Vasiliki Paraskevopoulou[2], Christos Kanellopoulos[3]

[1]Dept. of Analytical Laboratories, Division of Water Resources and Geothermal Energy, Hellenic Survey of Geology and Mineral Exploration (H.S.G.M.E.), Greece; [2]Laboratory of Environmental Chemistry, Dept. of Chemistry, School of Science, National and Kapodistrian University of Athens, Greece; [3]Dept. of Mineral & Mining Research, Division of Mineral Resources and Mining, Hellenic Survey of Geology and Mineral Exploration (H.S.G.M.E.), Greece

Antimony (Sb) is a critical element, frequently associated with complex ore deposits and mining waste (tailings), requiring accurate analytical protocols. This study focuses on the evaluation of various dissolution methods for determination of Sb in solid Certified Reference Materials. The primary aim is to identify the most suitable digestion technique for different sample matrices and to assess the possible impact of the matrix on Sb recovery and overall analytical accuracy. For this research, a comprehensive set of OREAS CRMs was utilized in order to encompass both, typical ore mineralizations and mining tailings, as well as a broad spectrum of Sb concentrations, varying from trace levels 40 mg/kg up to high-grade concentrations 3.5% w/w.

The dissolution approaches investigated include both microwave-assisted digestion and open-vessel acid digestion/evaporation in Teflon vessels. Different digestion times and extraction reagents were utilized, including mixtures of concentrated nitric acid and Aqua Regia. Each digestion experiment was performed in 10 replicates for each CRM, acid mixture and temperature program. Antimony was analyzed in the resulting digestion solutions using sensitive analytical techniques: Inductively Coupled Plasma – Optical Emission Spectrometry (ICP-OES) or Inductively Coupled Plasma – Mass Spectrometry (ICP-MS), depending on the anticipated Sb concentration to ensure optimal detection limits and precision.

The results demonstrate that simpler acid dissolution methods, such as HNO_3 and Aqua Regia, lead to low Sb recoveries across all tested CRMs. However, complete dissolution was achieved using aggressive multi-acid mixtures, such as the '3 Acids' method (HNO_3-HCl-HF), which consistently yielded recoveries of approximately 100% The '3 Acids + H_2O_2' technique also presented high efficiency, with recovery means typically in the 80-87% range (Table 1).

The adoption of a robust and efficient analytical protocol for antimony determination is crucial not only for accurate environmental monitoring but also for reliable resource assessment, given the presence of antimony mineralizations in Greece.

Table 1. Antimony Recovery (%) from Certified Reference Materials (CRMs) using Different Dissolution Methods
Note: 1 and 2 refer to temperature programs used. Temperature Program 1: The temperature was ramped up to 180 °C over 10 minutes and then held at 180 °C for an additional 30 minutes. Temperature Program 2: The temperature was ramped up to 180 °C over 15 minutes and then held at 180 °C for an additional 45 minutes.

Dissolution Conditions	OREAS 138 SEDEX TYPE Zn-Pb-Ag ORE		OREAS 630B Zinc Tailings (MMG Rosebery Mine, Australia)		OREAS 611B High Sulphidation Epithermal Au-Cu-Ag Ore		OREAS 292 Gold-Antimony Ore	
	Mean // (min-max) %Recovery	t-test	Mean // (min-max) %Recovery	t-test	Mean // (min-max) %Recovery	t-test	Mean // (min-max) %Recovery	t-test
HNO_3_1	7.1 // (7-8)	<100%	12.9 // (10-14)	<100%	22.0 // (14-33)	<100%	19.6 // (17-24)5	<100%
HNO_3_2	8.1// (7-10)	<100%	16.9 // (15-19)	<100%	19.8 // (19-21)	<100%	29.7 // (25-43)	<100%
Aqua Regia_1	13.3 // (12-14)	<100%	15.5 // (14-17)	<100%	18.9 // (18-19)	<100%	27.7 // (23-18)	<100%
Aqua Regia_2	17.7 // (14-20)	<100%	19.8 // (19-21)	<100%	21. 3 // (21-22)	<100%	29.6 // (26-32)	<100%
3 Acids (HNO_3-HCl-HF) dilution to 5% HNO_3	88.1 // (87-90)	<100%	99.0 // (89-106)	=100%	101. 0 // (91-107)	=100%	100.7 // (95-111)	=100%
3 Acids (HNO_3-HCl-HF) + H_2O_2, dilution to 5%HCl	73.4 // (68-80)	<100%	83.7 // (82-87)	<100%	87.5 //(80-98)	<100%	82.7 //(79-88)	<100%

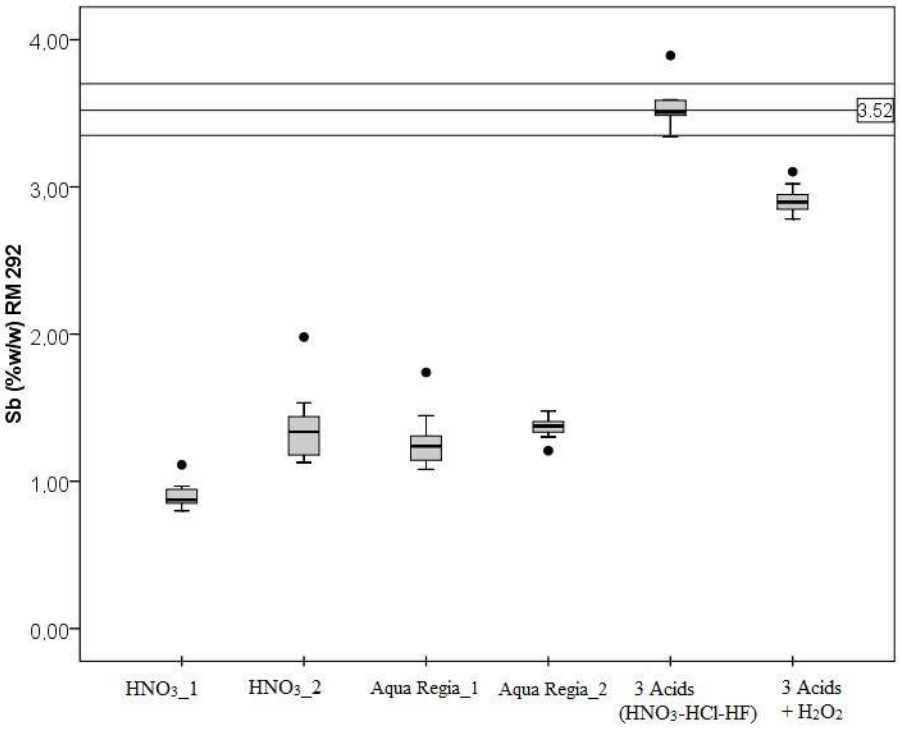


Figure 1. Antimony content (%w/w) boxplot from OREAS 292 Certified Reference Material using Different Dissolution Methods

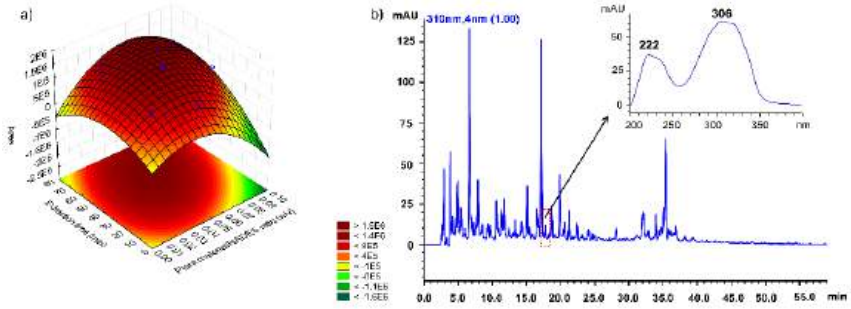
APC - D1 - P03

A sustainable strategy for high-yield resveratrol recovery from agro-industrial waste using optimized MAE-NADES

Mirella Thaisa Ferreira Ranzeti[1,2], Gabriela Cremasco[2], Daniel Rinaldo[1,2*]
[1]Institute of Chemistry - UNESP, Brazil; [2]Green Biotech Network, School of Sciences - UNESP, Brazil

Peanuts, the fifth-most-important oilseed globally, have significant socioeconomic relevance. Intensively cultivated in Brazil, the sixth largest exporter of peanut oil. Its cultivation generates significant agro-industrial waste, notably roots, which are a valuable source of resveratrol—a stilbene with potent antioxidant, anti-inflammatory, and anticancer properties.[1] To address the imperative for waste valorization and align with Green Analytical Chemistry (GAC) principles, this study aimed to develop an efficient and sustainable method for extracting resveratrol from *Arachis hypogea* root residue. A green chemistry strategy was employed, combining Microwave-Assisted Extraction (MAE) with Natural Deep Eutectic Solvents (NADES). Following an initial screening of six NADES, the lactic acid:glycerol (1:1, mol/mol) mixture with 20% w/w water (NADES N4) was selected due to its superior extraction performance. The MAE-NADES method was then rationally optimized using Design of Experiments (DoE; Figure 1), establishing optimal conditions of a plant material/NADES ratio of 1:20 (m/v; X1), a temperature of 60 °C (X_2), and 40 minutes of extraction (X_3).

Fig. 1. (a) Response surface of the significant variables (X_1 and X_3), and (b) the HPLC-DAD chromatogram of the validated method extraction.



The developed MAE-NADES protocol achieved a resveratrol yield approximately 15 times higher than the best conventional extraction methods using methanol/water or ethanol/water. Furthermore, the sustainability of the process was confirmed by the AGREE[2] (score 0.8, Figure 2) and GAPI metrics, demonstrating high adherence to green chemistry principles. This work provides an efficient, environmentally responsible, and scalable protocol for recovering high-value resveratrol from agro-industrial peanut root waste.

Fig 2. AGREE metric pictograms for (a) the developed method; (b) the ethanol:water method; and (c) the methanol:water method, respectively.

The authors gratefully acknowledge Marina Piacenti da Silva (Department of Physics, São Paulo State University – UNESP, Bauru) for lending the microwave digestor. This work was supported by the National Council for Scientific and Technological Development (CNPq, Conselho Nacional de Desenvolvimento Científico e Tecnológico) under grants #303887/2024-9 and the State of São Paulo Research Foundation (FAPESP, Fundação de Amparo à Pesquisa do Estado de São Paulo) under grants #2025/03036-3, #2025/06438-5, #2025/14225-1, and #2022/11628-0, Brazil.

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APC - D1 - P04
Sedimentation kinetic of a textile adhesive

Cátia Alves[1], Emanuele Bassani[1], Letícia Costa[1], Afonso Bangui[2], Miguel Alberto Pacheco[2], Lídia Gonçalves[2], Alfredo Castro[2], Miguel Pacheco[2], Artur Ferreira[1], Nuno Gama[1]
[1]CICECO – Aveiro Institute of Materials and University of Aveiro, Portugal; [2]Heliotextil, S. A. São João da Madeira, Portugal

An adhesive is any substance which, when applied to the surface of objects, bonds them together, providing resistance to their separation. Based on this premise, adhesives are used in various applications, such as in civil construction, packaging industry, automotive sector, medicine, or textile industry[1]. Most adhesives used in the textile sector consist of an aqueous resin combined with a hot-melt component, and screen printing is one of the most common methods for applying them[2]. However, solid hot-melts tend to settle over time, and phase separation frequently occurs, resulting in a loss of homogeneity and, consequently, a reduction in the adhesive's performance[3]. Consequently, this study aims to analyse the sedimentation kinetics of a water-based textile adhesive to gain a deeper understanding of the sedimentation process. Sedimentation kinetics were evaluated by monitoring the interface height over time, deriving velocity and concentration from polynomial fits, and validating the findings using the Kynch model. Tests with varying hot-melt concentrations (2–5%), particle sizes (0.25–1.00 mm), and water contents showed that higher hot-melt concentrations, larger particle sizes, and lower water content significantly reduce sedimentation velocity, resulting in improved suspension stability. The formulation containing 5 wt.% hot-melt, 1.00 mm particles, and 50% water exhibited the highest stability. In screen-printing tests, this formulation enhanced print uniformity, although the durability of adhesion still requires optimisation.

This work was funded by FEDER - Fundo Europeu de Desenvolvimento Regional funds through of Programa Inovação e Transição Digital in the scope of the project "CIRATEX – Circularidade aplicada a adesivos têxteis", COMPETE2030-FEDER-01159700, and was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

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APC - D1 - P05
Development of tools in chemical metrology for standardization of the analysis of Brazilian hops

Cleyryson S. Lima [1], Igor R.B. Olivares[2]
[1]University of São Paulo, Chemistry Institute (IQSC-USP), Brazil; [2]University of São Paulo, Chemistry Institute (IQSC-USP), Brazil

The implementation of a Quality Management System in analytical laboratories has become fundamental due to increasing regulatory requirements, intensified industrial competitiveness, and growing market demands[1,6]. ISO/IEC 17025 is internationally recognized as a benchmark for demonstrating the technical competence and experience of testing laboratories. In this context, Certified Reference Materials (CRMs) and Proficiency Testing (PT) are fundamental for evaluating the reliability, accuracy, and traceability of analytical results[1]. This study aims to develop a CRM containing the main compounds responsible for the sensory properties of Brazilian hops and apply this material in a proficiency test with four varieties representative of national production[3,6]. Hops (Humulus lupulus L.) are a strategic input for the brewing industry, often called the "soul of beer," as they directly influence aroma, flavor, bitterness, and foam stability. These sensory properties are mainly associated with α, β, and γ resins, as well as the essential oils present in hop cones[5]. Currently, analytical reference methods for hop characterization are predominantly developed by the American Society of Brewing Chemists (ASBC)[4]. In Brazil, the absence of specific technical standards, consolidated metrological studies, and Certified Reference Materials for hops limits the comparability and reliability of analytical results. As a preliminary step, samples of Brazilian hops were subjected to supercritical fluid removal with carbon dioxide (CO_2), resulting in a homogeneous material containing the compounds of interest[5]. The results showed adequate recovery and preservation of relevant chemical characteristics. The production of the CRM will follow the guidelines of ISO Guide 35:2020, including homogeneity and stability studies, characterization by GC-FID and GC-MS, and uncertainty estimation, contributing to metrological traceability, analytical reliability, and the competitiveness of Brazilian hops[2].

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APC - D1 - P06

Probing interfacial effects in bismuth(III) electroreduction using simple mercury-based electrodes

Agnieszka Nosal-Wiercińska[1], Alicja Pawlak[1], Sultan Yagmur-Kabas[2], Robert Pietrzak[3]

[1]Dept. of Analytical Chemistry, Institute of Chemical Sciences, Faculty of Chemistry Maria Curie-Sklodowska University, Poland; [2]Dept. of Chemistry and Chemical Processing Technologies Programs, Lapseki Vocational School, Çanakkale Onsekiz Mart University, Türkiye; [3]Dept. of Applied Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Poland

The electroreduction of bismuth(III) ions is a process strongly governed by interfacial phenomena. A key role in determining both the mechanism and kinetics of this process is played by adsorption at the electrode/solution interface, as well as by the formation of transient structures, so-called active complexes, resulting from interactions between depolariser ions and organic substances (the “cap-pair effect”). While complex electrode surface modifications are often effective in applied studies, they may obscure fundamental mechanistic relationships. Therefore, fundamental investigations benefit from the use of simple and well-defined electrode systems that allow direct assessment of the influence of the reaction environment on the course of the electrode process.

In this work, a comparative study of Bi(III) ion electroreduction was carried out in mixed aqueous-organic media containing low-molecular-weight alcohols differing in the position of the hydroxyl group. Experiments were performed using a classical hanging mercury drop electrode (HMDE) and a renewable thin-film silver amalgam electrode (R-AgLAFE). The use of the amalgam electrode enabled a significant reduction in mercury consumption while preserving key electrochemical properties characteristic of mercury electrodes (such as high surface reproducibility and a wide potential window) [1], in line with current trends towards more sustainable electrochemical methodologies.

The study employed a complementary set of electrochemical techniques.

The results confirm that the R-AgLAFE electrode is a useful and effective tool for fundamental studies of interfacial phenomena in mixed aqueous-organic systems, enabling the essential features of the electrode process to be revealed.

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APC - D1 - P07

Assessment of the crystalline state of polymorphic pharmaceutical active ingredients in a forced degradation study utilizing seven recommended methodologies: Application to carbamazepine

Nardjess Rim Laoufi[1], Farida Bouchenak[1], Khaled Sobhi[1], Abdeldjalil Lalaouna[2], Youcef Hadef[3]
[1]Faculty of pharmacy, Algiers, Algeria; [2]Dept. of Pharmacy, Constantine, Algeria; [3]Dept. of pharmacy, Annaba, Algeria

Introduction: Carbamazepine (CBZ) is an active pharmaceutical ingredient that can manifest in five crystalline forms. Among these, the commercial form (monoclinic III) is the only thermodynamically stable variant. The U.S. The Food and Drug Administration mandates that, owing to the polymorphic nature of CBZ, a polymorphism study must be conducted during stability testing. The objective of the stability study undertaken in this research was to assess the evolution of properties associated with the crystalline state of raw materials and evaluate their progression using appropriate methodologies.
Material and Method: A forced degradation study was conducted on five batches of distinct CBZ raw materials, adhering to the ICHQ1A and, Q1E Q6A guidelines. The materials were subjected to conditions of 40±2°C and 75±5% relative humidity over a period of six months. Samples were collected at five intervals: T0, T1, T2, T3, and T6. The samples were analyzed using infrared spectroscopy, melting point testing, X-ray diffraction (XRD), differential scanning calorimetry (DSC), thermogravimetric analysis, polarized light optical microscopy, and scanning electron microscopy.
Results: Among the seven techniques evaluated, XRD identified the emergence of the dihydrate form as early as T1 and the triclinic I form as early as T2 in four batches from the same manufacturer. In contrast, the final batch from the other manufacturer exhibited no additional forms. DSC revealed significant differences in the partial and overall crystallinities of the five batches at T0 and throughout the stability study. This indicates that the batches contained varying amounts of the amorphous phase, which is more soluble but less stable than the monoclinic III form.
Conclusion: XRD and DSC are the most pertinent techniques for examining the crystalline transformations of carbamazepine. XRD facilitates the observation of new crystalline phases, whereas DSC allows for the evaluation of the degree of crystallinity of the raw material.

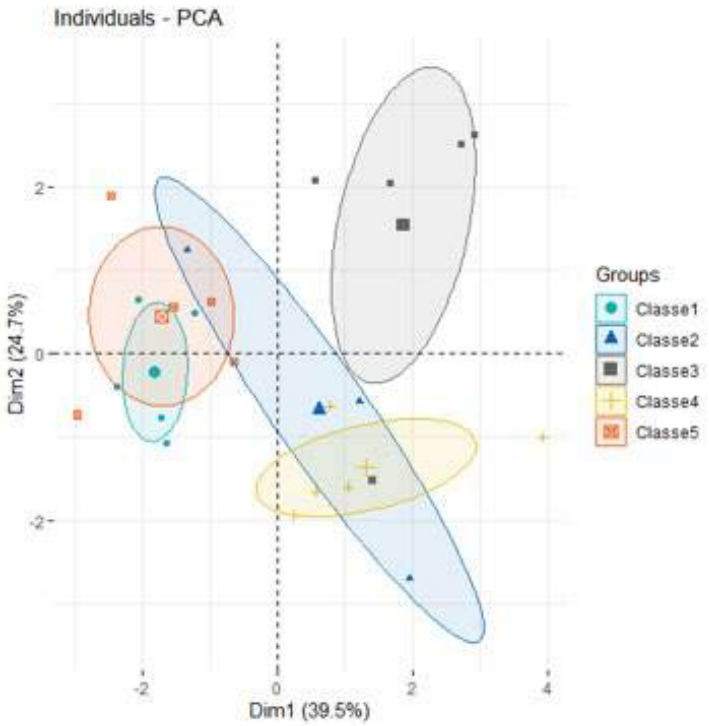

Fig. 1. illustrates the dispersion of crystalline properties across five batches, with classes 1, 2, 3, and 4 originating from the same manufacturer and class 5 sourced from a different manufacturer during the stability study.

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APC - D1 - P08

Predictive acoustic modelling of sustainable natural fibers and 3D-printed architected absorbers

Faouzia Tayari[1], Regina Silva[1], Rui Ribeiro[2], Pedro Pinto[2], Isabel Cardoso[2], Tiago Brilhante[2], Artur Ferreira[1], Vânia Teixeira[3], Nuno Gama*[1]

[1]CICECO/ESTGA and University of Aveiro, Aveiro, Portugal; *[2]Amplitude Acoustics – Acústica e Vibração, Lda., Portugal; [3]Lightenjin Iluminação, Águeda, Portugal*

The growing demand for sustainable noise-control solutions has intensified the need for materials that combine high acoustic absorption performance with environmentally responsible design. This study investigates two promising families of sound absorbers: bio-based natural fibers (hemp, raffia, textile waste, and several coconut variants) and 3D-printed structures from PLA and PLA bio-composites. The acoustic behaviour of all samples was characterized exclusively using the Microflown In-Situ Impedance Gun, enabling direct measurements under realistic boundary conditions. Afterwards, inverse modelling was employed to identify the key non-acoustic parameters governing sound propagation in porous media. For natural fibers, the Johnson–Champoux–Allard–Lafarge (JCAL) model accurately reproduced the measured absorption spectra and captured the complex pore networks intrinsic to lignocellulosic materials. For the 3D-printed absorbers, the Johnson–Champoux–Allard (JCA) model successfully predicted microstructural properties and revealed how geometric architecture and bio-filler reinforcement influence acoustic performance. The results demonstrate that natural fibers provide highly efficient and sustainable sound-absorbing solutions, while additively manufactured structures offer tunability and lightweight design possibilities beyond traditional materials. Overall, this work highlights the essential role of predictive acoustic models and in-situ measurement techniques in advancing the next generation of eco-designed porous materials.

Funding: This research was funded by FEDER – Fundo Europeu de Desenvolvimento Regional funds through of Programa Inovação e Transição Digital in the scope of the project “BiMAIS”, COMPETE2030-FEDER-01195100, and was developed within the scope of the project CICECO – Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

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APC - D1 - P09
ShinyCDS: An open-source R-based software for reproducible processing of chromatograms

Edouard Salingros[1]
[1]University of Liège, Gembloux Agro-Bio Tech, Belgium

The use of proprietary file formats and software for the storage and processing of chromatographic data is a well-known obstacle to interoperability, long-term readability and reproducibility. While numerous open-source software resources (e.g., packages and libraries) exist, their installation and use often require above-average knowledge and skills in coding and computer science. The most advanced, general-purpose, ready to use software with a graphical user interface (GUI) is likely the free base version of OpenChrom[1]. Yet, inspecting, editing and re-compiling OpenChrom source code (Java language) is not easy.
This poster presents *ShinyCDS*, an open-source program executing the application logic in R and using the package "shiny" to render a graphical user interface in a web browser. In its current state, *ShinyCDS* can read chromatograms supplied in .txt format, execute common signal smoothing algorithms, detect and integrate peaks, assign compounds based on retention times, quantify unknown samples based on calibration chromatograms and internal standards and export results in common tabular and spreadsheet formats. Complete processing methods can also be saved for reproducible analysis.
Beyond its functionalities related to chromatographic data processing, *ShinyCDS* can be regarded as a lever for digital sovereignty and transparency. Since R is one of the most popular programming languages for data analysis, *ShinyCDS* source code can be easily understood and edited to include new functionalities. The program can be executed offline on any computer having R and the required packages installed, or from any computer (even without R installed) connected to an open-source shiny server[3] (hosted on-premise and served through a local network or over the internet).

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APC - D1 - P10

Study of the stability and degradation of the LQM330 molecule active against the Chikungunya virus (CHIKV)

Clara Andrezza Crisóstomo Bezerra Costa[1], Johnnatan Duarte de Freitas[1], Edeildo Ferreira da Silva Júnior[2], João Xavier de Araújo Júnior[2]

[1]Federal Institute of Alagoas (IFAL) – Maceió Campus, Dept. of Chemistry, Multi-user Laboratory in Environmental Technologies; [2]Federal University of Alagoas (UFAL), Department of Pharmacy, Medicinal Chemistry Laboratory

The characterization of solids and liquids for drug and medicine development is essential to ensure the processing, transport, and storage of final products. Certain acrylamides are active against the Dengue (DENV) and Zika (ZIKV) viruses, exhibiting significant biological action and low toxicity in human cells; these substances are classified as organic molecules. In recent decades, a growing number of suspected cases of Chikungunya (CHIKV) infection has been noted—a disease that is often neglected due to symptoms similar to DENV and ZIKV. The study and characterization of active molecules are of great importance for therapeutic alternatives that remain unknown or underexplored. The objective of this work was to determine the thermal stability and degradation of the acrylamide LQM330, which is active against the CHIKV virus. The characterization of the molecule was performed using Thermogravimetry (TG), Differential Scanning Calorimetry (DSC), and Scanning Electron Microscopy (SEM). The TG curves demonstrated that the molecule is stable at different heating rates (10, 20, 30, 40, and 50 °C min^{-1}) with material stabilization in the range of 248.78 °C and a mass loss of 67.18%. The DSC curve provided data regarding the melting point of the molecule. The thermal decomposition profile of LQM330 presented exothermic events associated with the "curing" of the materials, as well as a small impurity peak. This technique also provided data on the purity of the molecule, which was in the range of 96.31%. The morphological aspects of the LQM330 molecule were heterogeneous, brittle, and clustered in general, with the exception of the samples at 600 °C (T600 °C), which presented whole, homogeneous cubic shapes. The high thermal stability of the LQM330 molecule confirmed that it is a promising candidate for the development of future potential medications against the CHIKV virus.

The authors would like to thank the Federal Institute of Alagoas (IFAL) and the Postgraduate Program in Environmental Technologies (PPGTEC/IFAL) for the support provided through their equipment and laboratory facilities.

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APC - D1 - P11

Characterization of the LQM330 molecule by high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC/MS) and fourier-transform infrared spectroscopy (FTIR)

Clara Andrezza Crisóstomo Bezerra Costa[1], Johnnatan Duarte de Freitas[1], Edeildo Ferreira da Silva Júnior[2], João Xavier de Araújo Júnior[2]

[1]Federal Institute of Alagoas (IFAL) – Maceió Campus, Dept. of Chemistry, Multi-user Laboratory in Environmental Technologies; [2]Federal University of Alagoas (UFAL), Dept. of Pharmacy, Medicinal Chemistry Laboratory, Brazil

The characterization of solids and liquids for drug and medicine development is essential to ensure the processing, transport, and storage of final products. Some acrylamides are active against the Dengue (DENV) and Zika (ZIKV) viruses, exhibiting significant biological activity and low toxicity in human cells; these substances are classified as organic molecules. The study and characterization of active molecules are of great importance for therapeutic alternatives that are still unknown or underexplored. The objective of this work was to characterize the LQM330 molecule using High-Performance Liquid Chromatography (HPLC), Gas Chromatography-Mass Spectrometry (GC/MS), and Fourier-Transform Infrared Spectroscopy (FTIR). The results showed that the LQM330 molecule presented a purity range between 92.50% and 99.81% via GC/MS and HPLC, respectively. UV-Vis spectra demonstrated a maximum absorption band in the ultraviolet-visible region around 220 to 335 nm for the LQM330 molecule; these results were confirmed by the HPLC technique through the absorption range at a wavelength of 254 nm. FTIR spectra demonstrated the presence of C=O stretching and N-H stretching, indicating the presence of amide and carboline in the infrared absorption bands. Therefore, the importance of complementary analytical techniques for the characterization of these substances is essential. Consequently, these techniques provided specific data for the LQM330 molecule, which can be further confirmed by other official techniques used in the pharmaceutical sector. This molecule is a promising candidate for the development of future potential drugs against the CHIKV virus.

The authors would like to thank the Federal Institute of Alagoas (IFAL) and the Postgraduate Program in environmental Technologies (PPGTEC/IFAL) for the support provided through their equipment and laboratory facilities.

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APC - D2 - P01
Silver and gold nanospheres for SERS-based detection of G-quadruplexes

Petra Petrović Popović[1], Adriana Kenđel[1], Nikša Krstulović[2], Tea Juračić[1], Snežana Miljanić[1]
[1]University of Zagreb Faculty of Science, Croatia; [2]Institute of Physics, Centre for Advanced Laser Techniques, Croatia

A prerequisite for surface-enhanced Raman scattering (SERS) is the adsorption of molecules onto or into close proximity with metallic nanoparticles.[1] While surface charge is essential for stabilizing plasmonic nanoparticles in suspension, it also strongly affects molecular adsorption at the nanoparticle surface. Consequently, SERS enhancement is favored when colloidal nanoparticles and target molecules carry opposite charges, whereas adsorption, and thus Raman scattering enhancement, is hindered or even suppressed when both possess the same charge. G-quadruplexes (G4s) are highly ordered nucleic acid structures formed within guanine-rich DNA and RNA sequences.[2] Due to their phosphate backbone, these structures are highly negatively charged. Owing to their biological relevance, particularly their involvement in regulating gene expression and suppressing tumor cell proliferation, G4 structures have been investigated using a variety of analytical techniques.[3] To assess the applicability of SERS spectroscopy for the detection of G4 structures, silver and gold nanospheres with different surface charges were prepared. Positively and negatively charged nanospheres were synthesized via chemical reduction reactions in aqueous media. Negative charge originated from citrate ions retained on the nanosphere surface following synthesis, whereas positive charge was achieved by coating the nanospheres with spermine. Additionally, silver and gold nanospheres were prepared by pulsed laser ablation, producing particles free of residual surface species from the synthesis process, yet carrying a slight negative charge. All prepared nanospheres were thoroughly characterized using UV/Vis/NIR absorption spectroscopy, zeta potential measurements, dynamic light scattering, and scanning electron microscopy. The physicochemical properties of the prepared nanospheres were correlated with their SERS efficiency for detecting the G4 structure formed by the telomeric DNA sequence d[$(TTAGGG)_4$] (Tel24). Despite their negative surface charge, citrate-stabilized silver nanospheres yielded the most intense SERS spectra, enabling effective monitoring of the DNA sequence folding.

Acknowledgments: This research was financially supported by the Croatian Science Foundation through the Project IP-2025-02-9095.

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APC - D2 - P02

Interactions of engineered silica nanoparticle-bound PFOA: Adsorption and toxicological effects on pulmonary health

Khianne Ed Miguel Pajarillo Orteza[1], Sheena Anne Henson Garcia[1], King Lun Yeung[1,2]
[1]Dept. of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Clearwater Bay, Hong Kong SAR, China; [2]Division of Environment and Sustainability, The Hong Kong University of Science and Technology, Clearwater Bay, Hong Kong SAR, China

Controlled-release fertilizers are critical due to environmental regulations limiting direct nitrogen application, which can contaminate water sources. Colloidal silica (SiO_2) shows promise for nutrient retention in topsoil, reducing nitrogen leaching. However, the introduction of nanomaterials into the environment raises concerns about their interactions with existing pollutants, such as microplastics and perfluoroalkyl substances (PFAS), particularly perfluorooctanoic acid (PFOA), known for its persistence. We investigated whether SiO_2 nanoparticles (SiO_2NPs) enhance PFOA toxicity or mediate its cellular effects. We conducted an adsorption experiment using 20 nm SiO_2NPs coated with PFOA at varying concentrations (5 µg/mL, 2.5 µg/mL, and 1.25 µg/mL). Samples were collected at multiple time points to assess the adsorption rate. All treatments reached a maximum adsorption of 20% within one hour, with varied desorption behaviors before equilibrium. TEM revealed that adsorbed NPs retained their size and shape post-adsorption and UV-treatment before use in biological assays. Exposure of various mammalian pulmonary cell lines (A549, Calu-3, NHBE) to PFOA/SiO_2NPs at 100 µg/mL approached the cytotoxic threshold (TC80) compared to the control (SiO_2 only), although it was found to be non-genotoxic via single-cell electrophoresis. We also compared the effects of SiO_2NPs, PFOA, and PFOA/SiO_2NP treatments at different concentrations, focusing on cell spheroidal size and growth behaviors, and surface protein alterations through qRT-PCR. Additionally, lung cells in an air-liquid interface (ALI) model were assessed for barrier integrity via luciferase assay. Proteomics examined the toxicity-related subcellular changes across the cell models. This comprehensive approach enhances our understanding of the interactions between SiO_2 nanomaterials and persistent environmental pollutants, informing strategies to mitigate their public health and environmental impacts.

Keywords: Silica nanoparticle, PFOA, cytotoxicity

APC - D2 - P04

Ratiometric fluorescence and chromogenic probe for ultra-trace detection of selected transition metal ions

Abrar Hussai[1,2], Sang Hyun Park[1,2]

[1]Advanced Radiation Technology Institute (ARTI), Korea Atomic Energy Research Institute, Jeongeup, Republic of Korea; [2]Radiation Science, University of Science and Technology, Daejeon, Republic of Korea

The increasing presence of toxic transition metal ions in environmental, biological, and aquatic systems has created a strong demand for simple, sensitive, and reliable analytical sensing methods. Among the available approaches, ratiometric fluorescence and chromogenic probes are particularly attractive because they allow both visual detection and accurate quantification. In this study, we describe the design and analytical performance of a heterocyclic symmetrical Schiff base derivative developed as a dual-mode ratiometric fluorescence and colorimetric probe for the selective detection of Co(II), Cu(II), and Hg(II) ions. The ligand was fully characterized using physical measurements, optical studies, NMR, FT-IR spectroscopy, and mass spectrometry to confirm its structure and photophysical behavior. Upon interaction with the target metal ions, the probe exhibited clear and reproducible changes in absorption and fluorescence spectra, accompanied by distinct visible color variations, indicating effective ligand–metal complex formation. In contrast, no noticeable chromogenic or spectral response was observed in the presence of other commonly encountered metal ions such as Na^{+}, Ag^{+}, Ni^{2+}, Mn^{2+}, Pd^{2+}, Pb^{2+}, Cd^{2+}, Zn^{2+}, Sn^{2+}, Fe^{2+}/Fe^{3+}, Cr^{3+}, and Al^{3+}, demonstrating the high selectivity of the sensing system. This selectivity is attributed to the favorable coordination environment and electronic compatibility between the ligand framework and the selected transition metals. Fluorescence titration experiments enabled quantitative evaluation of sensing performance, yielding detection limits of 2.92×10^{-8} M for Co(II), 8.91×10^{-8} M for Cu(II), and 4.39×10^{-3} M for Hg(II). Furthermore, Benesi–Hildebrand analysis confirmed stable complex formation, with association constants of 0.74, 2.52, and 13.89 M^{-1} for Co(II), Cu(II), and Hg(II), respectively. Overall, this work presents a straightforward and effective analytical platform for selective and ultra-trace detection of transition metal ions, highlighting its potential for practical applications in environmental monitoring and related analytical studies.

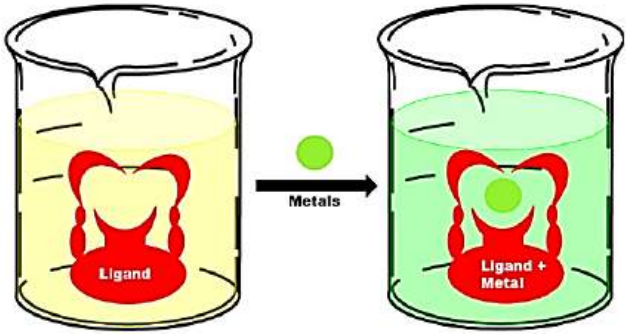

Fig.1. Schematic representation of the symmetrical ligands, showing the visible chromogenic response of the receptor solution before and after metal ion addition, along with the corresponding ligand–metal interactions.

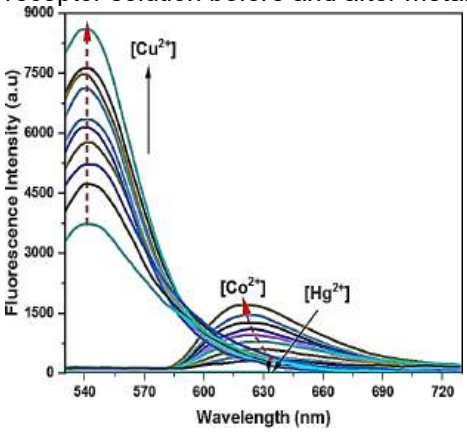

Fig. 2. Fluorescence titration analysis of probe alone and after incremental induction of $Co^{2+,}$ Cu^{2+} and Hg^{2+} salt solution.

APC - D2 - P06
Determination of antimony species and analysis in various food using ICP-MS

Yong-Kyoung Kim, Ji-Yeon Ham[1], Hye-Jin Cho, Eunji Choi, Ji-Woo Seo, Jin Sook Kim
[1]*Food Contaminants Division, National Institute of Food and Drug Safety Evaluation, Ministry of Food and Drug Safety, Republic of Korea*

Foods produced in areas impacted by antimony (Sb) pose significant health risks due to the uptake of toxic metalloids such as Sb. Given that the toxicity and bioavailability of Sb depend heavily on its chemical speciation—specifically the more toxic trivalent Sb (III) versus the less toxic pentavalent Sb (V)—accurate speciation analysis is essential. In this study, an analytical method using high-performance liquid chromatography coupled with inductively coupled plasma mass spectrometry (HPLC-ICP-MS) was developed and optimized. Using experimental design methodology, EDTA was selected as the optimal extraction reagent due to its superior extraction yield and compatibility with the mobile phase. The separation of Sb (III)- and Sb (V)-citrate complexes was performed on a PRP-X100 anion-exchange column using a mobile phase of 18 mmol EDTA, 16mM nitric acid and 4% methanol (pH 4.6). The proposed method demonstrated excellent analytical performance and satisfied CODEX performance criteria. The linear range of 0 – 2 ng/mL (r = 0.999) and a limit of detection (LOD) of 0.0014 mg/kg and 0.0009 mg/kg for both Sb (III) and Sb(V). Precision remained below 15%, and recoveries ranged from 84.8–108.7% for Sb (III) and 70.4–101.7% for Sb(V) in various representative foods. The method was successfully applied to analyze various food samples. These results suggest that the developed method is a reliable tool for monitoring Sb species in food and assessing associated health risks.

APC - D2 - P07

Thermodynamics studies of L-threonine in aqueous1-butyl-3-methylimidazolium chloride solutions over the temperature range *T* = (288.15-318.15) K

Tarnveer Kaur
Dept. of Chemistry, Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab, India

Amino acids as fundamental structural units of peptides and proteins have an important role in biological systems by affecting solubility, denaturation and activity of biomolecules. Study of these effects on volumetric properties of model compounds in the presence of electrolytes solutions provide information about solute-solvent and solute-solute interactions on biomolecules. Ionic liquids (ILs) as organic electrolytes and green solvents are composed of an organic cation and an inorganic anion which are liquid at ambient conditions. In the past decade, extensive investigations showed that the use of ILs as reaction media for processes involving biologically relevant compounds is promising in view of their successful application in kinetic resolution, biocatalysis, biosynthesis, separation and purification processes. The scope of this information is valuable to explore the interactions of amino acids in ILs. To reach this purpose, densities, ρ of L-threonine in water and aqueous 1-butyl-3-methylimidazolium chloride, $[BMIm][Cl]$ solutions of different molalities over the temperature range *T* = (288.15-318.15) K have been determined using vibrating-tube digital density meter (DMA 4500M, Anton Paar, Austria). The density data have been used to calculate the apparent molar volume, $V_{\emptyset}$, partial molar volume, V_2^o and partial molar volumes of transfer, $\Delta_{tr}V_2^o$. The V_2^o values of L-threonine in aqueous $[BMIm][Cl]$ solutions are higher than those in water and thus exhibit positive $\Delta_{tr}V_2^o$, which are indicative of strong interactions between L-threonine and $[BMIm][Cl]$. The volumetric interaction parameters, V_{AB} and V_{ABB} and hydration numbers, n_H have also been calculated to discuss the solute-solvent interactions occurring in these systems.

APC - D2 - P08

Controlling gold nanoparticles aggregation in continuous flow microreactor for robust production of ultrasensitive NIR SERS nanotags

Alexandre Verdin[1], Pierre Stiernet[2], Louise Lejeune[3], Jean-Christophe M. Monbaliu[4,5], Sophie Hermans[3], Gauthier Eppe[1] and Cedric Malherbe[1]

[1]Mass Spectrometry Laboratory, University of Liège, Belgium; [2]Center for Education and Research on Macromolecules (CERM), University of Liège, Belgium; [3]Institute of Condensed Matter and Nanosciences (IMCN), UCLouvain, Belgium; [4]Center for Integrated Technology and Organic Synthesis (CiTOS), University of Liège, Belgium; [5]WEL Research Institute, Belgium

Surface-Enhanced Raman Scattering (SERS) nanotags are highly attractive for bioanalytical applications due to their outstanding spectral selectivity and sensitivity[1]. Strong SERS enhancement relies on the formation of intense electromagnetic hot spots, typically generated between closely spaced plasmonic nanoparticles. In this context, the controlled assembly of nanoparticle aggregates represents an efficient strategy to maximize SERS performance.

We report a continuous-flow chemistry approach enabling the controlled synthesis of gold nano-aggregates optimized for near-infrared (NIR) SERS[2]. A two-stage microreactor platform was employed to induce aggregation of 30 nm gold nanoparticles using malachite green isothiocyanate (MGITC), simultaneously acting as Raman reporter and aggregating agent. Aggregation was subsequently quenched by introducing HS-PEG-COOH or HS-PEG-folic acid (FA), ensuring rapid stabilization of the nano-aggregates. Aggregation degree could be precisely adjusted by systematically tuning MGITC flow rate and residence time within the reactor. The resulting nano-aggregates were characterized using UV–Vis spectroscopy, dynamic light scattering (DLS), transmission electron microscopy (TEM), and SERS. The flow-based platform further demonstrated excellent reversibility, allowing real-time switching between different aggregation states during operation. Optimized nano-aggregates exhibited a 100-fold increase in SERS sensitivity compared to non-aggregated nanoparticles. Moreover, functionalization with HS-PEG-FA provided targeting capabilities toward cancer cells overexpressing folate receptors[3]. In cancer tissue imaging performed under 785 nm excitation, nano-aggregates produced high-contrast SERS maps, whereas conventional non-aggregated SERS tags failed to generate detectable signals.

This work introduces an on-demand, continuous-flow strategy for producing tailored SERS nanotags that combine enhanced signal intensity with biological specificity, offering strong potential for biomedical imaging and diagnostic applications.

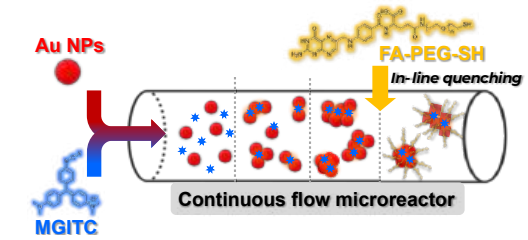

Fig. 1. Graphical abstract representing the general concept of this work.

Funding: Alexandre Verdin and Pierre Stiernet acknowledge funding from the F.R.S-FNRS (postdoctoral fellowship).

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APC - D2 - P09

Synergistic modulation of anticholinergic and antioxidant features of Alzheimer's disease drugs adsorbed on tunable graphene oxide surface

Pynskhemborlang T. Phanrang[1], Sivaprasad Mitra[1],
[1]Dept. of Chemistry, North-Eastern Hill University, India

The pursuit of drugs with multi-therapeutic functionality has intensified in recent years, particularly in the post–COVID-19 era. In the context of Alzheimer's disease (AD), growing evidence suggests that several FDA-approved AD drugs, such as huperzine A (HUP) and tacrine (TAC), possess intrinsic antioxidant activity.[1] This dual functionality can contribute to neuroprotection by mitigating oxidative stress–induced neuronal damage, enabling a more comprehensive approach to AD therapy. Enhancing these complementary properties through appropriate formulation strategies is therefore of considerable interest. Graphene oxide (GO) has emerged as an effective nano-interface for drug modulation. Adsorption of AD drugs on GO surfaces substantially enhances both their acetylcholinesterase (AChE) inhibitory efficiency and radical-scavenging activity.[2] Such findings establish GO not merely as a carrier capable of traversing the blood–brain barrier, but as an active surface that directly modulates drug functionality.

Systematic reduction of polar oxygen functionalities on the GO surface (viz. GO1, GO2 and GO3) induces linear enhancement in both AChE inhibition and antioxidant activity of the adsorbed AD drugs. For instance, HUP reduces the AChE hydrolysis rate (V_{max}) by 22%, 29%, and 32% in the presence of GO1, GO2, and GO3, respectively, while antioxidant activity increases by 14%, 19%, and 22% relative to the free drug. These enhancements originate from surface-induced electronic effects driven by controlled GO polarity, which strengthen drug-surface interactions and stabilize reactive intermediates involved in radical scavenging and enzyme inhibition. Overall, surface-tunable GO emerges as an effective platform for amplifying the multifunctional therapeutic potential of AD drugs and offers mechanistic insight into nanomaterial-drug interactions relevant to neuroprotective drug design.

Acknowledgements: Financial support from CSIR (CSIR-RA, award no. 323-560-6399/2k24/1), New Delhi, India, is gratefully acknowledged.

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APC - D2 - P10

Spacer-mediated interplay of triplet excitons in delayed fluorescent emitters

Soumya Ranjan Panda,[1] Dhananjaya Sahoo,[1] Apurba Lal Koner[1]
[1]Bionanotechnology Laboratory, Dept. of Chemistry, IISER Bhopal, India

Designing organic emitters that maintain efficient delayed fluorescence in the solid state remains a significant challenge for practical device applications.[1] Although both TADF (Thermally Activated Delayed Fluorescence) and TTA (Triplet-Triplet Annihilation) offer routes to recycle triplet excitons, their activation is highly sensitive to molecular packing, conformational freedom, and host–guest interactions in solid films.[2] Polymer matrices often introduce energetic disorder and restrict molecular motion, leading to the simultaneous presence of multiple emissive species such as locally excited states, charge-transfer states, and excimer/aggregate states.[3] Herein, we have designed two molecules for TADF and two for TTA by using naphthalimide (**NI**) derivative as an acceptor and n-phenyl carbazole (**PhCBZ**) or carbazole (**CBZ**) as a donor at 5,6-position of naphthalimide moiety. Thin films of the CBZ and PhCBZ-substituted naphthalimides doped in the poly(methyl methacrylate) (**PMMA**) matrix exhibit TADF emission and TTA-induced delayed emission, respectively. The subtle structural modification alters intermolecular p- p and CH- p interactions (**Fig. 1**), directing PhCBZ-substituted molecules toward a TTA pathway while CBZ-substituted analogues predominantly exhibit TADF.[4]

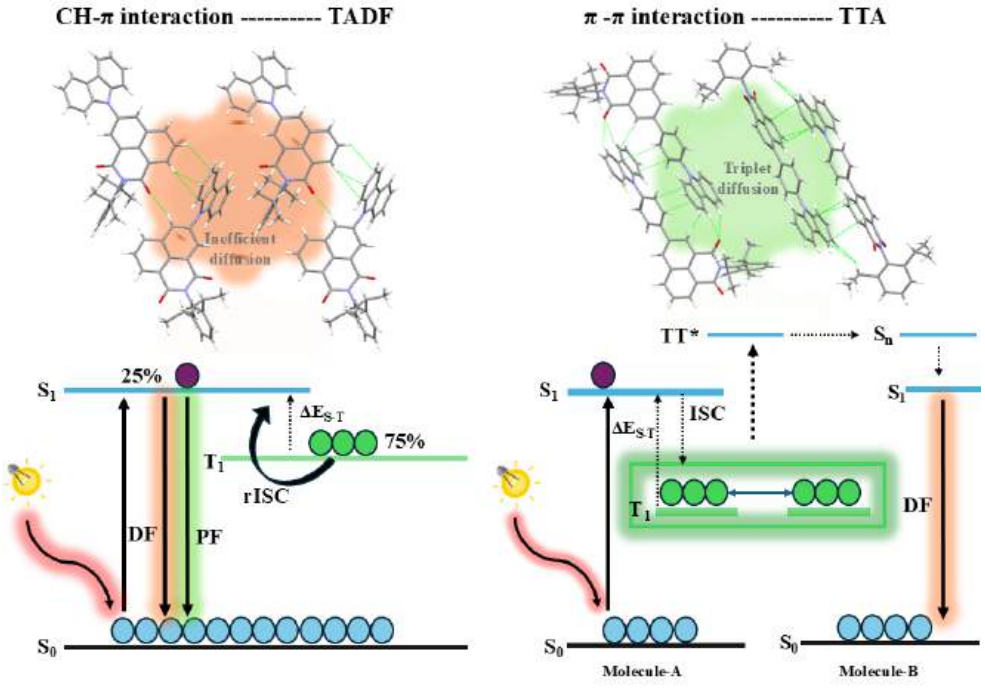

Fig. 1. Illustration of the TADF and TTA mechanisms, highlighting the intermolecular interactions responsible for the different delayed fluorescence (DF) pathways.

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APC - D2 - P11

Analytical strategy for speciation-resolved monitoring of labile arsenic using passive sampling and HPLC-ICP-MS

Vendula Smolíková[1], Lika Bakhturidze[1], Steven Goderis[1], Yue Gao[1], Martine Leermakers
[1]Vrije Universiteit Brussel (Archaeology, Environmental Changes and Geo-Chemistry), Belgium

Accurate evaluation of arsenic contamination requires analytical approaches that go beyond total concentrations, as arsenic toxicity and environmental behaviour depend strongly on chemical speciation. Nevertheless, regulatory monitoring still relies on dissolved or total arsenic measurements, providing limited information on the labile, potentially bioavailable species.

The Diffusive Gradients in Thin Films (DGT) technique enables *in-situ* preconcentration of labile trace elements and provides time-integrated measurements. However, its application to arsenic speciation remains limited due to the lack of species-selective sorbents[1]. Here, we present analytical strategy coupling passive sampling with chromatographic separation to enable speciation-resolved determination of labile arsenic.

The retention behaviour of environmentally relevant arsenic species – As(III), As(V), monomethylarsonic (MMA) and dimethylarsinic (DMA) acids – was evaluated using commonly applied DGT sorbents (ZrO_2, Metsorb (TiO_2), and Bayoxide E33 (FeOOH)). Although DMA uptake decreased at neutral to alkaline pH (≥8), all sorbents exhibited affinity for all tested species. This indicates that, in the presence of methylated arsenic, DGT-based inorganic arsenic measurements may be biased unless speciation is resolved.

To address this limitation, a strategy combining Bayoxide E33-DGT with HPLC-ICP-QQQ-MS was developed, building on previous work by Österlund et al.[2] Optimization focused on preserving species integrity during sorption and elution, ensuring eluate's chromatographic compatibility, and minimizing matrix interferences. Optimal performance was achieved using 1 mL of 1 M H_3PO_4 as DGT eluent, combined with pH adjustment and reduced injection volumes. Partial oxidation of As(III) and MMA observed during elution was reproducible and can be corrected mathematically.

This work provides a foundation for speciation-resolved monitoring of labile arsenic, supporting risk-based environmental assessment.

This work was supported by the Research Foundation Flanders (12AMZ24N, I002122N) and VUB Strategic Research.

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APC - D2 - P12

Thermotropic and thixotropic lipid based nanocarriers: Structure, rheology and phase behaviour

Giulia Gabbricci[1,2,3], Ilaria Clemente[1,2,3], Luigi Talarico[1,2,3], Agnese Magnani[1,2,3]

[1]Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy; [2]Center for Colloids and Surface Science (CSGI), Florence, Italy; [3]National Interuniversity Consortium of Material Science and Technology, Florence, Italy

The growing demand for effective, safe, and stable delivery systems in pharmaceutical and cosmetic application has driven increasing interest in lipid-based nanocarriers such as solid lipid nanoparticles (SLNs) and nanostructured lipid carriers (NLCs)[1]. In topical formulation, the efficacy and stability of the final product are not only determined by nanoparticles size, composition and encapsulation efficiency, but also by their structural and rheological properties. Indeed, the stability, physical appearance, and efficacy of nanoparticles-based products are strongly influenced by nanosystem bulk structuring and phase transitions of the nanosystems. Smart formulations capable of responding to external stimuli such as temperature and mechanical stress, represent a promising strategy to maximize performance while ensuring optimal product flow properties[2].

In this work, we developed thermotropic and thixotropic SLNs and NLCs dispersions for the encapsulation of bioactive molecules for topical delivery. A spontaneous and reversible transition from liquid to gel state was observed, which was accelerated by decreasing temperature, with recovery of the liquid state upon temperature increase or application of shear stress. Nanosystems size, surface charge and stability over time were investigated by Dynamic Light Scattering (DLS) and Zeta Potential measurements, revealing monodisperse populations ranging from 150nm to 300nm, high surface charge and good long term size stability. Rheological measurements performed at 20°C and 40°C showed a thixotropic behaviour and different dynamic viscosity. Small-angle X-ray scattering (SAXS) experiments performed at 20°C (gel like state) and 40°C (liquid state) revealed that gelation is associated with the formation of liquid crystalline structure with a lamellar organization, whereas at 40°C the nanoparticles exist in a fully dispersed liquid state. Differential scanning calorimetry (DSC) showed the lipid core melting events, while atomic force microscopy (AFM) and transmission electron microscopy (TEM) provided complementary insights into particle morphology and nanoscale organization.

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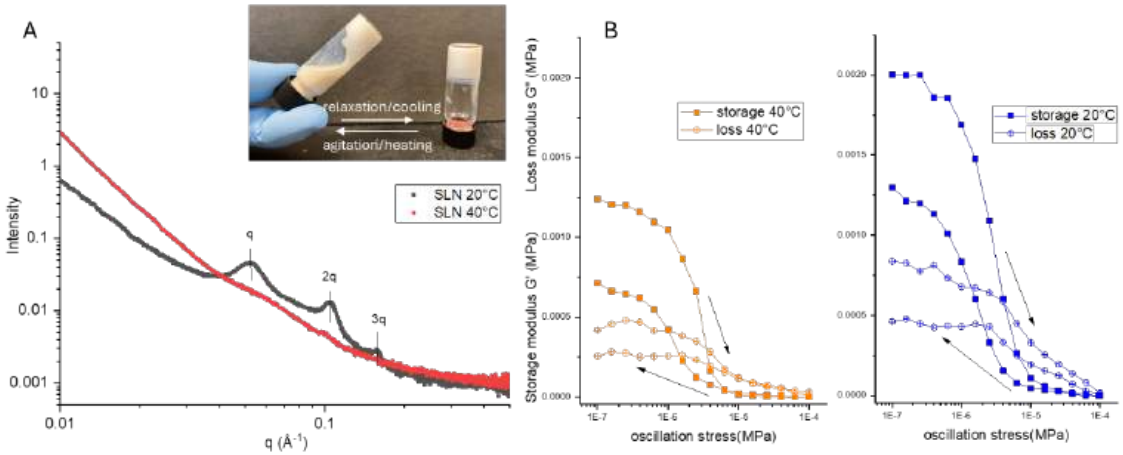

Fig. 1. a) SAXS measurement at 20°C and 40°C b) Viscoelastic behaviour upon oscillation stress/relaxation at 20°C and 40°C

APC - D2 - P13

Cyclodextrin-coumarin complexes as corrosion inhibitors of carbon steel 1020 in acid medium

Igor Zanetti[1], Luis Henrique Lacerda[1], Maria Eduarda Rocha[1], Victor. M. Paiva[1], Marcelle L. F. Bispo[2], Camilo H. S. Lima[1], Eliane D'Elia[1], Luiz Fernando B. Malta[1]

[1]Instituto de Química, Universidade Federal do Rio de Janeiro, Brazil; [2]Dept. de Quimica, Universidade Estadual de Londrina, Brazil

Coumarin derivatives are effective corrosion inhibitors for metals such as steel and aluminum in corrosive media, such as 1 mol L-1 HCl.1 The film adsorbed on the metal surface is formed mainly by the interaction of the carbonyl group of the molecule with the surface, capable of simultaneously inhibiting anodic and cathodic processes.1 However, its low solubility in aqueous media limits its use as a high-efficiency inhibitor. To remediate this, the use of cyclodextrins2 (CDs) as an additive allows the formation of a water-soluble supramolecular complex with the inhibitor owing to the amphiphilic property of CDs. In the present study, modified coumarin N-(2-bromophenyl)-3-carboxamide-coumarin (pcum, Figure 1) and alpha, beta, and gamma hydroxypropylated cyclodextrins (HPaCD, HPbCD, and HPgCD, respectively) were used. The complexes were synthesized using lyophilization (LIO), in which a mixture of coumarin and cyclodextrin in water was stirred for 24–72 h until solubilization, and then the solution was frozen overnight followed by a freeze-drying process; and mechanochemical method (MM), in which the pcum-HPCD physical mixture was subjected to ball milling for 12 h. Corrosion inhibition tests were performed in triplicate using gravimetric mass loss assays of 1020 carbon steel in 1 mol L^{-1} HCl. The inhibition efficiency (IE, Table 1) was 7.7% for pcum alone (170 ppm), and values between 47.2 and 70.7% were obtained for the HPgCD and HPaCD complexes (having 50 ppm pcum), respectively, synthesized via lyophilization. In contrast, the samples obtained via MM did not exhibit inhibition efficiency owing to complex incipient formation. The use of cyclodextrins alone resulted in low IE values (9-24%). These results demonstrated CD complexes to significantly increase the pcum inhibition efficiency against corrosion of carbon steel in acid.

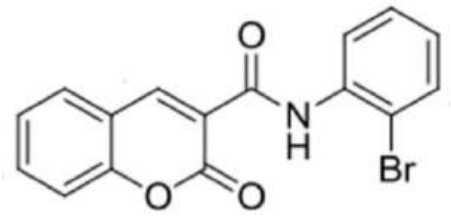

Fig. 1. Structural representation of *N*-(2-bromophenyl)-3-carboxamide-coumarin (pcum)

Table 1: Inhibition Efficiency (IE) results obtained for LIO (lyophilized) and MM (mechanochemical method) cyclodextrin complexes with *N*-(2-bromophenyl)-3-carboxamide-coumarin (pcum)

Sample	IE(%)	SD(%)
pcum*	7.7	0.5
HPaCD	26.4	1.1
LIO-HPaCD	70.7	0.4
MM-HPaCD	0.0	-
HPbCD	23.8	3.5
LIO-HPbCD	68.4	3.0
MM-HPbCD	0.0	-
HPgCD	9.4	1.6
LIO-HPgCD	47.2	5.4
MM-HPgCD	0.0	-

*170 ppm assay

The authors acknowledge CAPES, CNPq and FAPERJ for financial support.

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APC - D3 - P01

Determination of dopant elements in optical crystals with solid sampling high-resolution continuum source graphite furnace atomic absorption spectrometry

Dániel Csontos[1]*, Krisztián Lengyel[1], László Kovács[1], Szaller Zsuzsanna[1], László Bencs[1]
[1]Wigner Research Centre for Physics, Hungary

High-purity lithium niobate ($LiNbO_3$) crystals are attractive hosts for nonlinear optical applications, and therefore, are the subject of extensive physical−chemical studies. These crystals are usually grown from melts of metal oxides using Czochralski or high-temperature top-seeded solution growth (HTTSG) methods. The optical properties of the crystal can be tuned with specific dopants added as oxides to the starting materials before crystal growth. Bismuth is an outstanding dopant, exhibiting real-time holographic display and long-lived photochromic signals in lithium niobate. Potassium is used in an oxide form during growth as a flux material, therefore it can be incorporated into the crystal host's lattice and negatively influences the physical-chemical properties.

In this study, methods were developed for the characterization of these dopants, using high resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS-GFAAS) with solid sampling. Samples were dispensed into graphite boats and weighed on a microbalance. Conditions were optimized by varying the parameters of the graphite furnace heating program and dispensing different masses of the pulverized crystal samples into the graphite boats.

Analytical lines of Bi I 227.658 nm and K I 404.414 nm were selected for the method. In solid sampling GFAAS, calibration is a challenging task, due to the lack of solid standards of matching and well-known elemental composition. Consequently, standard solutions were applied for calibration, based on the standard addition method for the solid sample. For this purpose, two means of calibration were utilized, i.e., common standard addition and the three-point estimation standard addition (Fig. 1). The analytical results obtained with both calibration methods showed good agreement. The LODs were found to be 0.32 and 0.53 µmol/mol, respectively. The Bi and K content of the crystal samples were in the range of 3.9-19.4 µmol/mol and 0.45-1.12 µmol/mol, respectively. The accuracy of the methods was verified against solution introduction HR-CS-GFAAS.

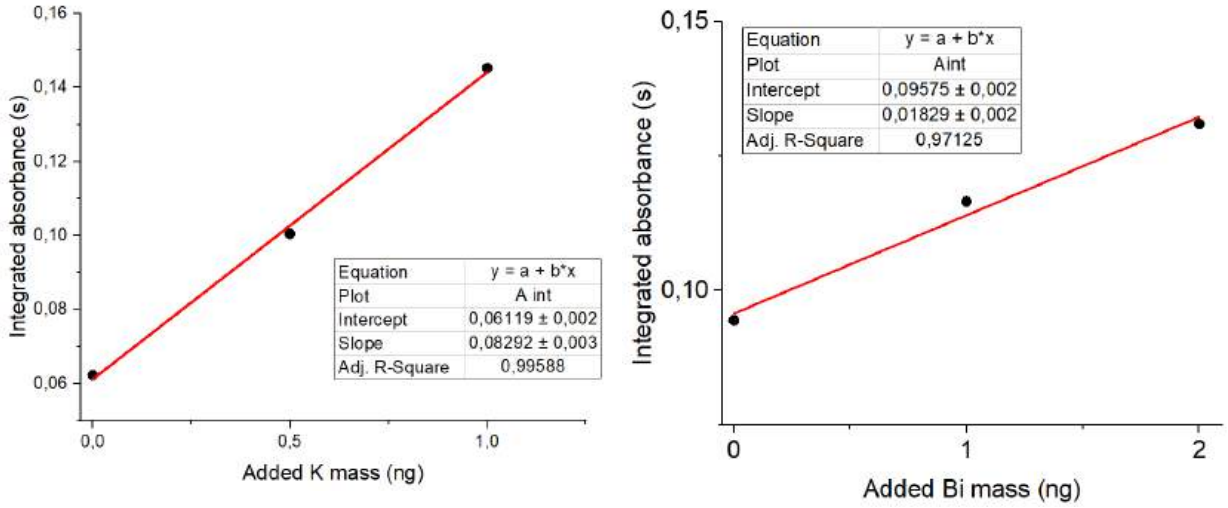

Fig. 1. Three-point estimation standard addition calibration of Bi and K in a lithium niobate sample

APC - D3 - P02

Studies on the improvement of the electrolyte cathode atmospheric glow discharge for environmental monitoring purposes

Dániel Csontos[1], Márk Medve[1], Ákos Kuntár[1], László Bencs[1]
[1]Wigner Research Centre for Physics, Hungary

Electrolyte cathode atmospheric glow discharge (ELCAD) is a DC microplasma, which was developed for optical emission spectrometry (OES) monitoring of environmental samples.[1] A common example of their application is the on-line monitoring of metal contaminants (e.g., Cd, Cu, Ni, Pb, Zn) in natural and wastewaters.[2] In principle, the ELCAD technique utilizes the direct introduction of certain aqueous solution (electrolyte) samples without the need for any additional sample dispersion unit (e.g., nebulizer), common in atomic spectroscopy techniques (e.g., inductively coupled plasma OES, flame AAS/OES). However, this simplicity and the small plasma volume of ELCAD is a drawback, which gives rise to various spectral and non-spectral interferences.[3] For instance, due to the direct introduction of aqueous solutions, the plasma is saturated with water vapour and related plasma species (e.g., OH-radicals), which cause the appearance of intensive OH-bands in the emission spectra (Fig. 1).
In this work, some novel findings of the ELCAD-related research are presented, e.g., the use of alternative atmospheres (e.g., Ar) around the glow discharge, chemically modified aqueous media for the standard/sample electrolytes to counteract interference effects and/or to enhance the emission intensities of analytes. The optimization of the conditions (sample solution pH, sample flow rate, plasma observation height, anode–cathode distance, etc.) will be discussed. The results will be compared in connection with regular solution media applied in ELCAD and alike plasma spectroscopy methods. The analytical results will be highlighted through some examples of direct sample analysis, including natural waters.

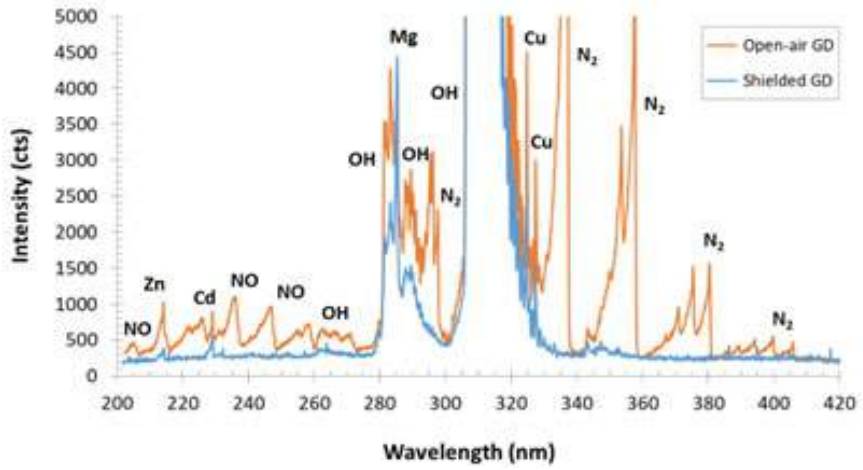

Fig. 1. Spectra of ELCAD recorded with an open-air and a shielded GD-cell (50 ppm Cd, Cu, Zn, Mg in HCl, pH 1.53).

APC - D3 - P03

Artificial intelligence-assisted optimization of an HPLC method for the determination of levetiracetam and piracetam

Murat Soyseven[1]*, Göksel Arli[2], Zeki Serdar Ataizi[3], Burcu Sezgin[4]
[1]Dept. of Medical Services and Techniques, Yunus Emre Vocational School of Health Services, Anadolu University, Türkiye; [2]Dept. of Analytical Chemistry, Faculty of Pharmacy, Anadolu University, Türkiye; [3]Dept. of Neurosurgery, Eskişehir Yunus Emre State Hospital, Türkiye; [4]Dept. of Environmental Protection Technologies, Eskişehir Vocational School, Eskişehir Osmangazi University, Türkiye

Levetiracetam (LEV) is a modern antiepileptic drug with broad clinical application in seizure management. Piracetam (PIR) is a neuroactive nootropic agent that enhances cognitive performance and is frequently used in neurological therapies[1-6]. Accurate analytical monitoring of these compounds requires robust and optimized chromatographic methods. In recent years, studies integrating artificial intelligence with HPLC methodologies have increasingly emerged[7]. This study presents an artificial intelligence (AI)-assisted approach to the development of a high-performance liquid chromatography (HPLC) method for the simultaneous determination of LEV and PIR. Chromatographic parameters, including mobile phase composition, flow rate, and temperature, were experimentally varied to generate a dataset representing analytical system behavior. Machine learning models were trained using experimental chromatographic data to describe nonlinear relationships between operational parameters and analytical responses such as retention time, resolution, and analysis duration. The trained models were employed as predictive tools to estimate analytical performance under untested experimental conditions. The AI system enabled multi-objective optimization by simultaneously considering chromatographic separation efficiency and operational performance. Using this predictive framework, optimal chromatographic conditions were obtained with fewer experimental trials, reducing experimental workload and resource consumption. The predicted optimal conditions were experimentally verified, demonstrating good agreement with model predictions. The study demonstrates that artificial intelligence can function as a decision-support tool in chromatographic method development rather than replacing experimental validation. Integrating data-driven modeling with laboratory experimentation allows rational optimization of analytical methods and improves efficiency. The proposed workflow indicates that combining chromatography and artificial intelligence provides a promising strategy for modern analytical chemistry, offering faster method development, reduced trial-and-error experimentation, and improved analytical reliability.

Acknowledgements: This research was funded by Anadolu University Scientific Research Projects Fund Commission Project No: 3112. The authors thank to Yunus Emre Vocational School of Health Services Research Laboratory in Anadolu University.

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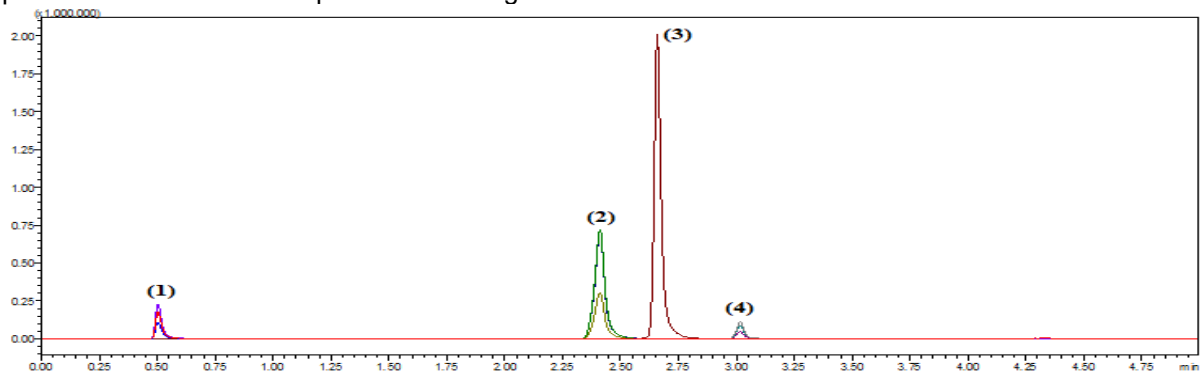
APC - D3 - P04

LC-MS/MS method development and validation for clinical pharmacokinetics and therapeutic drug monitoring of potassium-competitive acid blocker vonoprazan-based triple therapy for H. pylori in human plasma

Ahmed Hemdan[1], Naser F. Al-Tannak[1], Hani M. Hafez[2], Abdullah Aldasem[3] and Ibrahim Khadra[3]
[1]Kuwait University, Kuwait; [2]Al-Esraa University, Iraq; [3]University of Strathclyde, UK

A newly FDA-approved triple therapy for Helicobacter pylori eradication combines vonoprazan (VPN), a potassium-competitive acid blocker, with amoxicillin (AMX) and clarithromycin (CMN). This study reports the development and full validation of a rapid, selective, and sensitive LC-MS/MS method for simultaneous quantification of these drugs in spiked human plasma. Sample preparation employed a straightforward liquid–liquid extraction (LLE) procedure. Chromatographic separation was completed within 5 minutes using a Phenomenex Kinetex C18 column (100 × 4.6 mm, 2.6 µm) with a gradient elution of 0.1% formic acid in water and acetonitrile. Diazepam served as an internal standard, and mass spectrometric detection was performed in multiple reaction monitoring (MRM) mode with positive electrospray ionization. The method demonstrated excellent linearity across the tested ranges (2–100 ng/mL for AMX and CMN; 5–100 ng/mL for VPN). Both intra- and inter-day precision and accuracy complied with FDA bioanalytical validation guidelines, with relative standard deviations and errors below 15%. Mean absolute recoveries exceeded 93% for all analytes. Greenness assessment using the AGREE tool confirmed the method's environmental friendliness. Overall, the validated LC-MS/MS method provides a rapid, reliable, and eco-friendly approach for simultaneous determination of VPN, AMX, and CMN in human plasma, supporting its potential application in clinical pharmacokinetic and therapeutic monitoring studies.



Total ion chromatogram (TIC) chromatograms for Amoxicillin (1), Vonoprazan Fumarate (2), Clarithromycin (3), and Diazepam (4) at 10 ng/mL.

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APC - D3 - P05

Forensic characterization of cannabis in vape products and labeled products seized in two court cases: A case study

Hashan Weragala, Piyumi Wijethunge, Kanchana Rathnapala, Udani Kathriarachchi, Asiri Ipalawatta
Narcotic Section, Government Analyst's Dept., Sri Lanka

The rapid emergence of electronic cigarettes containing cannabis-derived constituents presents significant analytical and interpretative challenges for forensic laboratories. Illicit vape products incorporating psychoactive substances like Δ^9-tetrahydrocannabinol (THC), cannabidiol (CBD), and cannabinol (CBN) from *Cannabis sativa L.* pose growing public health and regulatory concerns. This necessitates robust analytical workflows for their accurate identification in seized materials.

Case Report including Results: This report details the forensic examination of two court productions submitted to Sri Lanka's Government Analyst's Dept., which included vape products and labeled joint materials. A systematic analytical workflow was employed, comprising visual examination, presumptive testing with Fast Blue B reagent, and thin-layer chromatography (TLC) for screening, followed by conclusive gas chromatography–mass spectrometry (GC–MS) for definitive confirmation.

Visual inspection revealed brown, viscous liquids within the vape devices and dried herbal material in the joints. Presumptive testing with Fast Blue B yielded a characteristic red coloration, indicating phenolic cannabinoids, while TLC analysis showed results consistent with cannabinoid reference standards. The definitive GC–MS analysis confirmed the presence of Δ^9-THC, CBD, and CBN in all samples. Furthermore, a terpene profile rich in limonene, linalool, β-caryophyllene, and α-humulene supported a natural cannabis origin. The detection of glycerol triacetate (triacetin), a common e-liquid additive, exclusively in the vape liquids confirmed their deliberate formulation for vaping.

Conclusion: The combined analytical approach provided definitive forensic evidence of natural cannabis constituents in both vape liquids and joint materials. These findings highlight an emerging forensic and regulatory challenge, underscoring the critical need for enhanced monitoring and analytical preparedness in forensic laboratories to address the proliferation of these products, thereby ensuring public safety and supporting regulatory enforcement.

Keywords: Vape products; Δ^9-THC; cannabinoids; GC–MS.

APC - D3 - P06
Silver nanoparticle synthesis using a deep eutectic solvent and green tea

Mohammad Pouya Ashrafzadeh[1], Emma Smith[1]
[1]Dept. of Chemistry and Forensics, School of Science and Technology, Nottingham Trent University, UK

There are environmental and health hazards associated with conventional organic solvents used in metal nanoparticle (MNP) synthesis; Deep Eutectic Solvents (DESs) are a sustainable alternative and an appealing medium for green chemistry. In traditional MNP synthesis, toxic stabilizers such as cetyltrimethylammonium bromide, sodium dodecyl sulfate, and polyvinylpyrrolidone are used to provide electrostatic or steric repulsion.[1] However, DESs can play multiple active roles in MNP synthesis, simplifying the process and reducing the need for additional reagents.

This research employed a DES composed of betaine and glycerol (1:3) first to extract natural compounds from green tea and then to synthesize silver nanoparticles (AgNPs) using the extracted tea and silver sulfate. The tea extract was analyzed using UPLC-UV to quantify caffeine and gallic acid, both crucial in AgNP synthesis. MNP optical properties were characterized using UV-Vis spectroscopy, and the hydrodynamic diameter in aqueous suspension was measured by DLS. The size and morphology of the AgNPs were examined by TEM, while synthesis efficiency was determined by ICP-MS.

UPLC analysis allowed optimization of the extraction conditions of 90 °C and 75 minutes. The AgNPs synthesis using the DES-assisted green tea extract was optimized and the resultant particles were comprehensively evaluated. The effect of country of origin of green tea on the AgNP synthesis was investigated. AgNPs synthesized from Aldi green tea leaves under optimized conditions revealed a λ_{max} at 432 nm (**Figure 1A**), with a mean particle size of 19.6 nm (**Figure 1B**) measured by UV-Vis spectroscopy and TEM, respectively.

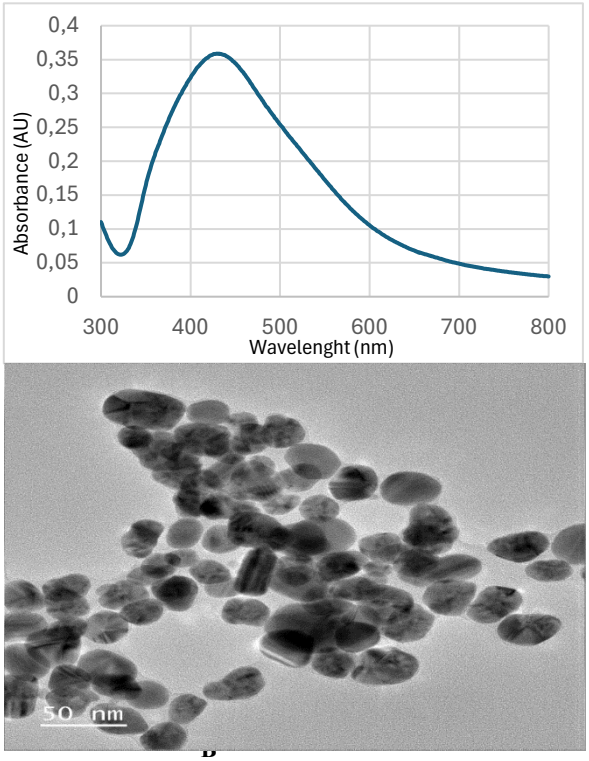

Fig. 1. (A) UV-Vis spectrum and **(B)** TEM image of AgNPs synthesized using 1 mL of extracted Aldi green tea, 3 mL of Bet:Gly (1:3) DES, and 0.025 g of silver sulfate at 90 °C for 75 minutes under stirring.

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APC - D3 - P07

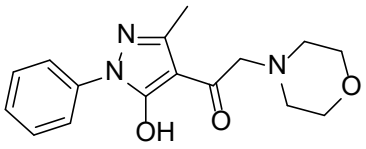
Green twist to solvent extraction and separation of metallic species with elfin chelating ligands

Maria Atanassova*, Lama Mzek, Nina Todorova

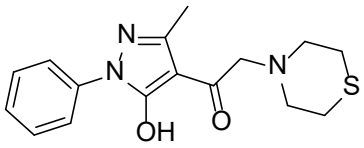
[1]*University of Chemical Technology and Metallurgy, Dept. of General and Inorganic Chemistry, Sofia, Bulgaria*

Email: ma@uctm.edu

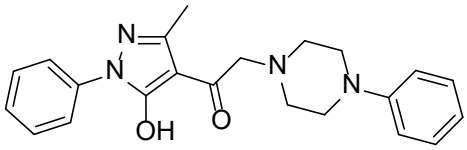
The competitive solvent extraction of various metal species in the periodic table by a series of ligands, tested for the first time, composed of N-heterocyclic receptors with variable ring size and one β-dicarbonyl fragment have been conducted to get a snapshot of their efficacy. The effect of heteroatoms in the substituent on the extraction performance and selectivity of this type of chelating extractants with equivalent binding sites but an unsymmetric backbone due to differing coordination environments has been evaluated. The effect of chemical nature of the organic liquid phase on the extraction process was also discussed: ionic liquids (IL, $[C_1C_nim^+][Tf_2N^-]$) or typical organic diluents. The superiority of the IL medium has been demonstrated. Nevertheless, the coordination capacity of the chelating agents is somehow meticulously dependent on the oxidation state of the extracted chemical element. The extraction capacity and selectivity of ligands towards lanthanoids were found to decrease on going from HL6 and HLO to $HLNC_6H_5$ and HLS. Generally, the decrease of extraction efficiency for compound HLS in comparison with other investigated molecules in an IL medium could be attributed to its solubility characteristics because in chloroform this ligand shows better extraction properties than others. The separation factors between adjacent metals of 4f-series and iron towards other metal ions have been assessed. Furthermore, EPR, Raman and DTA-TG-MS spectroscopies have been used to study the extracted d- and f-chelate complexes in the obtained extracts in IL solutions: Gd^{3+} and Fe^{3+}.



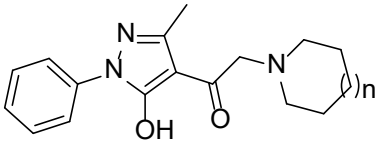
HLO



HLS



$HLNC_6H_5$



HL5 - n=0
HL6 - n=1
HL7 - n=2
HL8 - n=3

Funding: The research leading to those results received funding from the Bulgarian Science Fund: Grant Agreement № КП-06-Н69/5(2022), "*Green twist to synergistic solvent extraction and separation of rare earth metals"*.

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APC - D3 - P08
Drug release performance of amphiphilic polymeric micelles and cross-linked micelles

Ayşegül Özbal[1], Vural Bütün[1]
[1]Eskisehir Osmangazi University, Turkey

Micellar systems formed through the self-assembly of amphiphilic polymers have attracted significant attention due to their remarkable potential in drug delivery applications. Although polymeric micelles offer several advantages, including enhanced solubility of hydrophobic drugs, controlled release behavior, and biocompatibility, their structural instability under varying pH, temperature, or concentration conditions remains a major limitation. To overcome these challenges, chemical modification and cross-linking strategies have been widely employed to improve micellar stability and performance under physiological conditions. Accordingly, numerous studies in the literature have focused on the design and application of cross-linked amphiphilic polymeric micelles as robust and efficient carriers for drug delivery systems [1–3].
In the present study, a triblock copolymer, poly[(ethylene glycol) methyl ether methacrylate]-*b*-poly[(2-(dimethylamino)ethyl methacrylate]-*b*-poly[(2-(diisopropylamino)ethyl methacrylate] (PEGMEMA-*b*-PDMA-*b*-PDPA), was successfully synthesized. The amphiphilic copolymer was characterized by proton nuclear magnetic resonance spectroscopy and gel permeation chromatography. Micellar solutions were obtained by adjusting the pH of the block copolymer solution, while cross-linked micelles were prepared through the cross-linking of the inner PDMA-corona. The hydrodynamic diameters of the micelles and cross-linked micelles were determined using dynamic light scattering. The *in vitro* release behavior of the model drug dipyridamole was evaluated in phosphate buffer solution at pH 7.4. The results demonstrated that both noncross-linked and cross-linked micellar systems exhibit favorable characteristics, highlighting their potential applicability as effective drug delivery platforms.

The authors gratefully acknowledge the financial support provided by Scientific and Technological Research Council of Türkiye (GN: 123C505)

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APC - D3 - P09

Influence of silane-based monolayers on the stability and transformation of β-glycine using SHG microscopy

Selam Verbert[1], Olivier Deschaume[2], Stijn Van Cleuvenbergen[1]
[1]KU Leuven campus Kortrijk, Belgium; [2]KU Leuven campus Leuven

Controlling nucleation and polymorphic outcomes remains a key challenge in pharmaceutical crystallization. Various polymorphs of the same compound can exhibit distinct solubility, stability and bioavailability, so preventing unwanted polymorphic transition is crucial for ensuring drug quality, efficacy and safety[1,2]. Glycine serves as an ideal model for such studies due to its well-characterized polymorphs at ambient conditions (α-glycine, β-glycine and γ-glycine). It is well known that the least stable β-glycine can be formed under kinetically controlled conditions (e.g. at low supersaturation, antisolvent addition or confined crystallization)[3–6]. However, this polymorph is particularly difficult to isolate, as it rapidly converts into the thermodynamically stable α-glycine via solution-mediated transformation[7,8]. Here, we investigate how interfacial chemistry can modulate the kinetic landscape of glycine crystallization using silane-based monolayers bearing different terminal functional groups ($–NH_2$, –pyridyl, –F), alongside hydroxyl rich piranha cleaned substrates. β-glycine was crystallized via evaporative microdroplet confinement with methanol as anti-solvent. Second Harmonic Generation (SHG) microscopy was used for real-time, spatially resolved monitoring of polymorphic distribution and transformation. As a symmetry-sensitive technique, SHG provides intrinsic contrast between the non-centrosymmetric SHG active β form ($P2_1$) and the centrosymmetric SHG-silent α form ($P2_1/n$), allowing direct visualization of phase transformation kinetics at the solid-liquid interface[9].

Our findings reveal that crystal size distribution and the stability of β-glycine strongly depend on the surface chemistry of the functionalized substrate. Hydrophilic surfaces capable of forming strong hydrogen bonding ($–NH_2$ and –OH) extended the lifetime of β-glycine, likely through stabilizing its polar crystals faces and raising the energetic barrier for solution-mediated transformation, in contrast to rapid conversion on a hydrophobic fluorinated surface. Furthermore, 3D SHG imaging revealed spatial heterogeneity with SHG active β domains and SHG inactive α domains coexisting in individual crystals. Polarization-resolved SHG microscopy was also performed on selected SHG active crystals to gain deeper insight into crystal symmetry and molecular orientation. By combining P-SHG with 3D SHG imaging, polymorphic distribution and transformation pathways could be directly correlated with interfacial chemistry.

S.V. acknowledges support from the Fonds Wetenschappelijk Onderzoek (FWO) with n° g086522n.

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APC - D3 - P10

Ion mobility high-resolution mass spectrometry (IM-HRMS) – An emerging technique facilitating the analysis of environmental contaminants and their metabolites

Lidia Belova[1], Maosen Zhao[1], Mikel Musatadi[1,2], Maarten Roggeman[1], Giulia Poma[1], Fatima den Ouden[1], Alexander L.N. van Nuijs[1], Adrian Covaci[1]

[1]Toxicological Center, University of Antwerp, Antwerp, Belgium; [2]Dept. of Analytical Chemistry, University of the Basque Country (UPV/EHU), Leioa, Spain

Ion mobility high-resolution mass spectrometry (IM-HRMS) presents an advanced separation technique with applications vastly increasing in recent years. It allows the separation of ions based on shape and size, providing an additional separation dimension. From measured mobilities, collision cross section (CCS) values can be calculated providing an additional identification parameter in HRMS-based suspect screening. These advantages are of special interest for the identification of environmental contaminants in exposomics studies, often facing complex sample matrices and low annotation confidence due to limited coverage of emerging contaminants by existing reference spectral libraries.

This presentation describes two of our recent IM-HRMS applications in the analysis of emerging environmental contaminants. The first study focused on the utilization of CCS values for improved compound annotation in indoor dust samples collected in Flemish kindergartens. Despite increasing use of alternative plasticizers, phthalates remained among major annotated contaminant classes showing the highest detection frequencies and semi-quantified concentrations. Detected phthalates displayed extensive homologue series with side chains ranging between C_1 and C_{12}. Annotations confidence of homologue series was vastly improved based on CCS-*m*/*z* trendlines describing the relationship between CCS value and mass-to-charge (*m*/*z*) ratio. Homologue series showed characteristic trendlines with CCS values of suspect phthalate homologues falling within the 90th percent confidence interval calculated for the CCS-*m*/*z* trendline (Figure 1).

The second study focused on the use of a human liver microsome based *in vitro* model for the identification of metabolites of quaternary ammonium compounds – another major class of contaminants observed in the indoor environment. Characteristic changes in CCS values following metabolism reactions were observed and confirmed *in vivo* after the analysis of human urine samples. This confirmation improved the annotation confidence of metabolites and is expected to facilitate metabolite annotations for other contaminant classes.

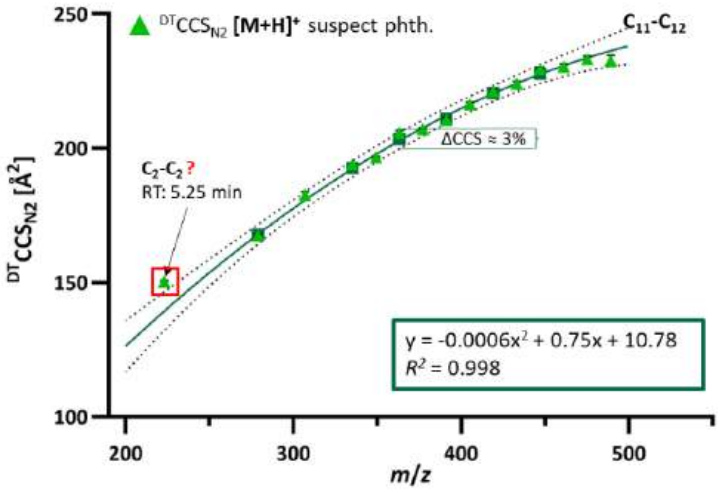

Fig. 1. CCS-*m*/*z* trendline describing the relationship between collision cross section (CCS) value and mass-to-charge (*m*/*z*) ratio. Dark-green squares represent CCS values calculated from phthalate reference standards. The corresponding CCS-*m*/*z* trendline was fitted using a 2nd order polynomial function for which the equation and correlation coefficient are displayed in the dark-green box. The 90th percent confidence interval is shown with dotted lines. CCS values obtained for suspect phthalates are displayed in light green. Datapoints falling outside the confidence interval were identified as false positive annotations (marked in red).

APC - D3 - P11
Synthesis and crystalline structure of diaquabis (5-methylthiazole-2-carboxylate-κ2N,O) cobalt (II)

S. N. Kamolov, B. T. Ibragimov
Institute of Bioorganic Chemistry Academy of Sciences of the Republic of Uzbekistan

Cobalt (II) acetate tetrahydrate (0.249 g, 1.0 mmol) was dissolved at room temperature in 2 ml of deionized water until complete dissolution. At the same time, 5-methylthiazole-2-carboxylic acid[1] (0.286 g, 2.0 mmol) was dissolved in 4 ml of absolute ethanol at a temperature of 60°C. The two transparent solutions were gradually combined under constant stirring. The resulting mixture was filtered through a 0.45 μm membrane filter. The filtered solution was left in an open container at room temperature (298 ± 2 K) for slow evaporation. After 10 days, green monocrystals suitable for X-ray analysis were formed. The product was separated by filtration, washed with cold ethanol, and air-dried. The yield (relative to cobalt) was 80%.

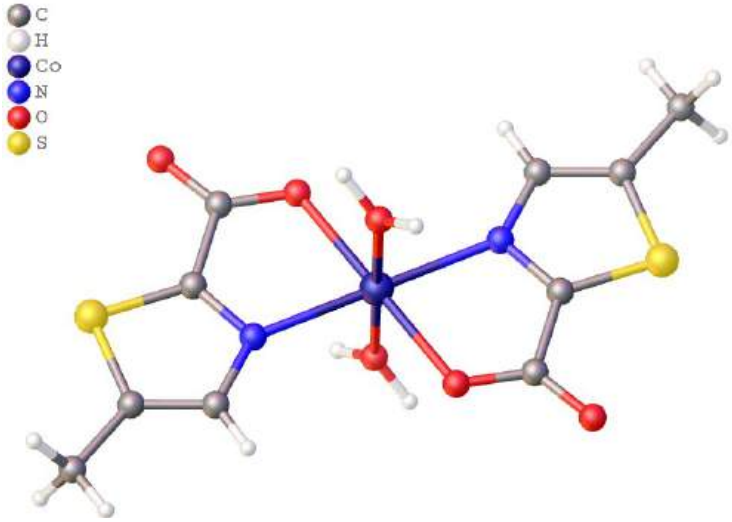

Fig. 1. Molecular structure of diaquabis (5-methylthiazole-2-carboxylate-κ2N,O) cobalt (II)

The substance crystallizes in a monoclinic P21/c space group, with four formula units in the unit cell. The central cobalt (II) ion is located in a slightly distorted octahedral-shaped coordination medium. It is bonded to two nitrogen atoms (Co-N 2.126 (6) Å) and four oxygen atoms of two 5-methylthiazol-2-carboxylate ligands: two from monodentate carboxylate groups (Co-O 2.133 (5) Å) and two from bound water molecules (Co-O 2.062 (4) Å). The carboxylate groups are monodentately coordinated, and the thiazole rings are located almost in the same plane as the coordination plane.
The crystal structure was determined using Cu Kα radiation at a temperature of 293 (2) K. The data were collected on an Xcalibur Ruby diffractometer[2]. The structure was solved by the charge flipping method and refined to the values of R1 = 0.1029 (I ≥ 2σ (I)) and wR2 = 0.2800 (all data).
Gratitude This study Uzbekistan. Supported by research grant number FL-9524115091 of the Institute of Bioorganic Chemistry of the Academy of Sciences.

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APC - D3 - P12

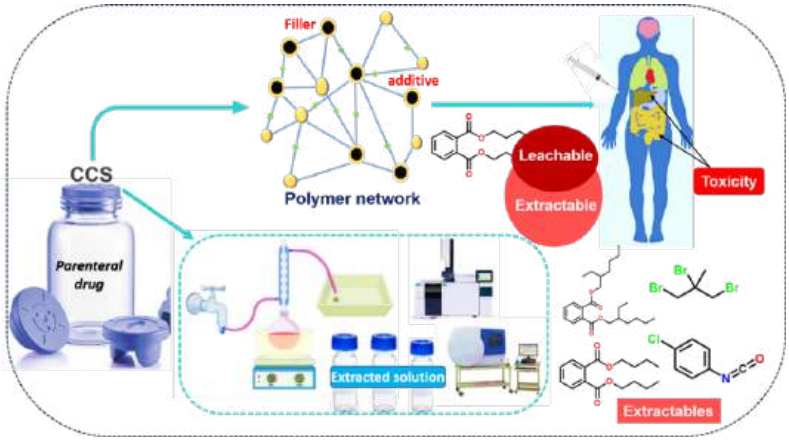
Comprehensive analytical evaluation and risk assessment of elastomeric container closure systems for biologics and small molecule parenteral drugs

Angana Pan, Ashutosh Kumar
Dept. Of Bioscience and Bioengineering, Indian Institute of Technology Bombay, Mumbai, India

Despite of assuming the chemical inertness of container closure system, bromobutyl stoppers can release extractable and leachable into the formulation that poses significant toxicological risk to human health and it is more concern with the parenteral drugs which bypass first pass metabolism. There is no standardized analytical platform for comparative evaluation of varying stopper size, composition, and surface engineering. This study aims to evaluate the extractables and leachable from different commercially available bromobutyl based rubber stopper by a systematic, orthogonal analytical methods like GC-orbitrap/MS, ICP-AES and 1H NMR to represent the worst-case scenario. Extraction was performed in aqueous solvents at pH 2.5 and 9.5, and in hexane, following USP ⟨1663⟩ and ⟨1664⟩ guidelines. A safety-based Analytical Evaluation Threshold (AET) was calculated for each stopper type, and real-world leachable migration was assessed in two model parenteral drug products biphasic insulin and 2% xylocaine under accelerated aging conditions simulating full shelf-life exposure.

A total of 17, 45, 9, and 18 volatile compounds were identified from RS I–RS IV, respectively, all are below their AET level. Among detected semi volatiles across RS I-RS IV by liquid injection GC-orbitrap/Ms, phthalate esters (dibutyl phthalate, DEHP, DIBP), phenolic antioxidants (2,4-di-tert-butylphenol, BHT), and long-chain hydrocarbons were identified across stopper grades. The most prominent two componenet leached from CCS of biphasic insulin are 2,4-di-tert-butylphenol (up to 12.98 µg/mL) and dibutyl phthalate (up to 7.41 µg/mL) and which are also exceeded respective AET level of 0.935 µg/mL under both accelerated aging condition and normal storage condition. In contrast, aqueous based small molecule drug (xylocaine 2%) leached very less number of compounds. This observation highlighted the role of formulation matrix particularly for biologic samples contains different excipient causes the more leachable migration. Elemental impurities remained below ICH Q3D-based thresholds under all conditions, with the exception of boron in RS I and RS III under acidic extraction. This study demonstrates that stopper composition, size, surface treatment, and extraction pH simultaneously influence the E&L risk profile. The integrated analytical strategy provides a robust framework for chemical characterization and toxicological risk assessment of elastomeric CCS, supporting informed material selection and regulatory decision-making for injectable drugs.

Keywords: Elastomeric container closure system; Extractables and leachables; Parenteral drug safety; GC-Orbitrap MS/MS; ICP-AES; Analytical evaluation threshold.



APC - D4 - P01
A polymer-based surface functionalization strategy for DNA immobilization on gold electrodes

Lorenzo Zarini[1,2], Paolo Bergese[1], Dario Brambilla[2]
[1]Università degli Studi di Brescia, Italy; [2]National Research Council of Italy, Italy

Surface functionalization is a critical step in the development of electrochemical DNA biosensors. Gold electrodes are widely used due to the well-established Au–SH chemistry, which enables the immobilization of thiolated DNA probes. However, thiol-based strategies often require time-consuming probe activation and suffer from limited long-term stability, as the Au–S bond is weaker than covalent linkages and prone to desorption and oxidation processes [1]. Here, we present a polymer-based coating strategy to rapidly and simply functionalize gold electrodes for DNA probe immobilization. The polymer was successfully applied to gold surfaces, The polymer was successfully applied to gold surfaces, as confirmed by electrochemical impedance spectroscopy. As shown in Figure 1, a marked increase in charge transfer resistance (Rct) was observed after polymer coating and subsequent DNA probe immobilization, indicating effective surface functionalization. Importantly, the polymer coating did not significantly alter the double-layer capacitance of the electrode, while providing antifouling properties. Overall, this approach enables a simple and robust functionalization of gold electrodes via hydrophobic interactions, offering a versatile platform for DNA-based electrochemical biosensing.

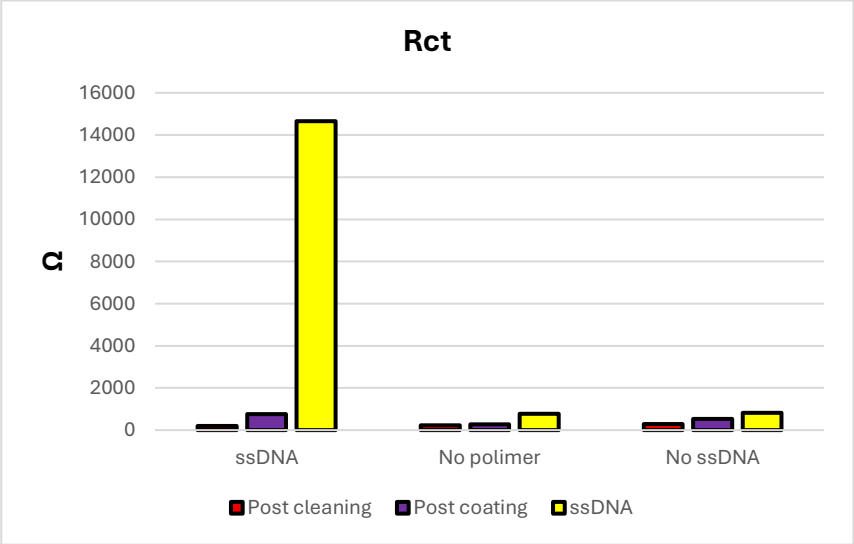


Fig. 1. Comparison of the charge transfer resistance (Rct) after surface functionalization.

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APC - D4 - P05
Exciton spatiotemporal imaging: From classical diffusion to quantum correlations

Shibin Deng[1]
[1]*Ultrafast Electron Microscopy Laboratory, The MOE Key Laboratory of Weak-Light Nonlinear Photonics, School of Physics, Nankai University, China*

Carrier dynamics are a key determinant of semiconductor device performance. However, studying carrier dynamics in nanometer/femtosecond scales under multi-physical field conditions is highly challenging. To overcome this bottleneck, we developed a wide-field transient optical microscope compatible with multiple physical fields. It achieves 300 fs time resolution, 30 nm spatial accuracy, and 10^{-5} OD sensitivity under 4 K, electric field, and 1 fps frame rate conditions. With this technology, we first realized optical imaging of the ultrafast transport process of excitons in two-dimensional perovskite materials[1], measuring their exciton diffusion rate and exciton annihilation coefficient. Further, we extended our field of view to the Moiré superlattice of two-dimensional transition metal dichalcogenides with strong correlation effects[2]. In this material, carrier behavior is no longer merely a classical diffusion process but is significantly influenced by quantum correlation effects. The strong long-range dipole repulsion between excitons leads to a "freezing" phenomenon in the dynamic behavior of the exciton Mott insulator, lasting up to 70 nanoseconds. This challenges the classical theory of repulsive forces dispersing particles and highlights the unique properties of quantum transport. These findings not only expand our understanding of exciton dynamics in low-dimensional materials but also provide new insights and theoretical foundations for the development of quantum information technologies and efficient optoelectronic devices.

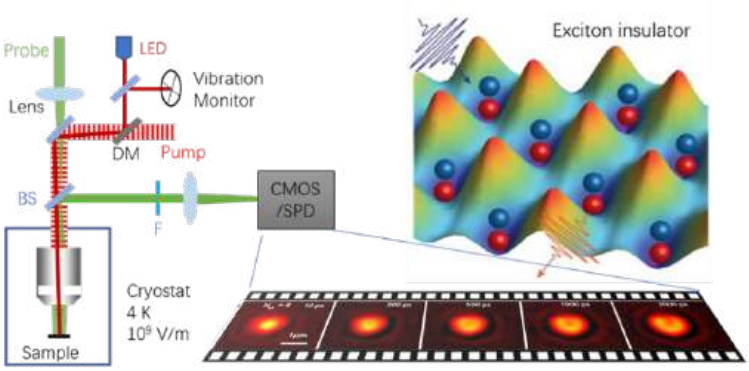

Fig. 1. Transient optical imaging of exciton dynamics.

Keywords: Transient absorption microscopy, transient fluorescence, exciton dynamics, Van der Waals heterostructures, interface interactions

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APC - D4 - P06

Untargeted UHPLC–IMS–M metabolomics reveals genotype-dependent chemical diversity among avocado varieties

María Gemma Beiro-Valenzuela[1], Lucía Olmo-García[1], Isabel López-Alcázar[1], Paula Jiménez-Mora[1], Sara Rodríguez-Rodríguez[1], Carmen María Sánchez-Arévalo[1], Romina Pedreschi[2], José Jorge González-Fernández[3], José Ignacio Hormaza[3], Alegría Carrasco-Pancorbo[1]

[1]University of Granada, Spain; [2]Pontificia Universidad Católica de Valparaíso, Chile; [3]Institute for Mediterranean and Subtropical Horticulture (IHSM La Mayora-UMA-CSIC), Spain

The global avocado market is largely dominated by the Hass variety due to its desirable sensory attributes, resistance to transport, extended postharvest shelf life, and the ease of monitoring ripening through characteristic skin colour changes. However, numerous less-studied avocado varieties exist and may represent promising alternatives in terms of agronomic performance, nutritional value, and opportunities for product diversification. A comprehensive understanding of the compositional differences among these varieties is essential before considering their potential introduction into commercial markets. In this context, metabolomic approaches provide powerful tools for the comprehensive characterization of fruit composition and for exploring metabolic variability associated with genetic background.

This study investigated the metabolomic profiles of 31 avocado varieties using an untargeted approach based on UHPLC–IMS–MS/MS. The varieties were classified into three groups according to their genetic background: *Hass* mutations, *Hass* descendants, and non-related varieties. Methanolic extracts obtained from freeze-dried mesocarp samples were analyzed using a UHPLC–timsTOF platform. The incorporation of collision cross section (CCS) values provided an additional molecular descriptor, enhancing annotation confidence through comparison with in-house spectral libraries, public databases, and in silico–predicted CCS values.

More than 100 metabolites were tentatively identified across all samples, including sugars, organic acids, amino acids, nucleosides, vitamins, and phenolic compounds (e.g., phenolic acids and flavonoids), as well as other metabolites relevant to fruit quality and nutritional value. Multivariate statistical analysis revealed distinct clustering patterns associated with genetic origin. Non-related varieties were widely dispersed across the PCA scores plot, indicating a high degree of metabolic diversity. In contrast, Hass mutations and Hass descendants formed compact, well-defined clusters clearly separated from the remaining varieties. Supervised PLS-DA models showed good fit and predictive performance, enabling the identification of discriminant metabolites responsible for class separation and suggesting their potential as genetic markers.

APC - D4 - P07

Postharvest storage and on-tree maturation drive distinct carbohydrate signatures in *hass* avocado

María Gemma Beiro-Valenzuela[1], Irene Serrano-García[1], Sara Rodriguez-Rodriguez[1], María Virginia Moreno-Tovar[1], Antonio Martín-Reyes[1], Carmen M Sánchez-Arévalo[1], Romina Pedreschi[2], Lucía Olmo-García[1], Alegría Carrasco-Pancorbo[1]

[1]University of Granada, Spain; [2]Pontificia Universidad Católica de Valparaíso, Chile

Avocado (*Persea americana* Mill.) is widely appreciated for its culinary and nutritional value. However, meeting the increasing global demand often relies on imported fruit that undergoes prolonged cold storage during transport. As a climacteric fruit, avocado ripens after harvest, and non-structural carbohydrates play a central role in this process. Despite their importance, the biochemical mechanisms governing carbohydrate dynamics during ripening and postharvest handling remain only partially understood.

This study evaluated how postharvest management influences the carbohydrate profile of *Hass* avocado mesocarp at edible ripeness by comparing prolonged cold storage with extended on-tree maturation. Approximately 125 fruits were harvested and stored under controlled temperature and humidity conditions in refrigerated chambers to simulate typical transport logistics. At 10-day intervals, subsets of fruits were removed from cold storage and allowed to ripen at room temperature until reaching edible ripeness. In parallel, freshly harvested avocados were collected from the trees at each time point and ripened under the same conditions to represent domestic supply scenarios. Five biological replicates, each consisting of five fruits, were analyzed per time point. Freeze-dried mesocarp samples were extracted using ultrasound-assisted solid–liquid extraction with a 60:40 (v/v) ethanol–water mixture, and the resulting extracts were analyzed by hydrophilic interaction liquid chromatography coupled with mass spectrometry (HILIC–MS).

The results revealed that cold-stored avocados exhibited a progressive accumulation of seven-carbon (C7) sugars, particularly perseitol and *D*-mannoheptulose. In contrast, fruits that remained longer on the tree accumulated higher levels of six-carbon (C6) sugars, including glucose, fructose, and sucrose. Principal component analysis (PCA) confirmed a clear separation between cold-stored and freshly harvested samples, highlighting the strong influence of postharvest conditions on avocado carbohydrate metabolism.

These findings provide new insights into how harvest timing and storage practices shape avocado metabolic composition, offering valuable guidance for improving postharvest management, optimizing supply chains, and enhancing fruit quality.

APC - D4 - P08
Surfactant-free microemulsions in surface cleaning

Ann-Christin Seidl[1], Eva Mueller[1], Werner Kunz[1]
[1]*Institute of Physical and Theoretical Chemistry, University of Regensburg, Germany*

Classical microemulsions are transparent, thermodynamically stable liquid systems composed of two immiscible phases, stabilized by amphiphilic molecules commonly referred to as surfactants. These molecules accumulate at the oil–water interface, lowering the interfacial tension and enabling the formation of oil-in-water, bicontinuous or water-in-oil structures.[1]
Beyond conventional systems, nanostructured single-phase solutions can be obtained without surfactants by incorporating hydrotropes. Unlike surfactants, hydrotropes are relatively small molecules with limited amphiphilic properties. Consequently, they neither form micelles in an aqueous solution nor create ordered interfacial films at the oil–water interface.[2,3] In ternary mixtures, these conditions can lead to the formation of surfactant-free microemulsions (SFMEs), which occur within the monophasic region above the phase boundary. The composition of these systems affects the observed structural regimes, with oil-in-water-like organizations typically associated with the so-called pre-Ouzo region.[4]
The nanostructuring in SFMEs is characterized by highly dynamic behavior and comparatively weak interfacial stabilization. Consequently, these systems exhibit pronounced mesoscale fluctuations and a high degree of structural flexibility. This combination of characteristics makes SFMEs a promising, environmentally friendly alternative for a variety of applications. In the context of surface cleaning, a detailed understanding of their dynamic structuring is essential to clarify their influence on cleaning efficiency and the underlying mechanisms.

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APC - D4 - P09
Characterization of tristyrylphenol ethoxylate surfactants

Clara Ernst[1], Eva Müller[1], Werner Kunz[1]
[1]Institute of Physical and Theoretical Chemistry, University of Regensburg, Germany

Surfactants comprise a broad class of amphiphilic compounds with applications like household products or industrial processes. A large proportion of their overall consumption occurs in industry, where their performance must be precisely tailored through structural design to meet specific functional requirements.[1]
Tristyrylphenol ethoxylates are nonionic surfactants distinguished by an extended aromatic core and a variable ethylene oxide chain length. While they are mainly employed in agrochemical formulations[2], their structural characteristics also indicate potential in fields such as pigment and dye processing[3], petrochemistry, and materials science. The pronounced aromatic moiety enables interactions with π-conjugated systems of other aromatic compounds, which may enhance the solubilization of such poorly water-soluble molecules. In particular, these surfactants can disrupt intermolecular π–π stacking, allowing subsequent solubilization via their hydrophilic segments.
However, these surfactants remain insufficiently characterized in the literature. Therefore, their fundamental physicochemical properties and solubilization mechanisms are systematically investigated using techniques such as UV–Vis spectroscopy, NMR and DLS measurements, complemented by measurements of surface tension, foaming behavior, rheology, and phase behavior in binary and ternary systems containing hydrophobic and aromatic solutes.

Acknowledgements: The authors thank Syensqo France for providing their tristyrylphenol surfactants for this study.

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APC - D4 - P10

Development and optimization of lipid nanocarrier systems for agri-food biowaste

Ginevra Vigni[1,2], Alessandro Donati[1,2], Claudia Bonechi[1,2], Raffaello Nardin[1,2], Agnese Magnani[1,2,3], Gemma Leone[1,2,3]

[1]University of Siena, Italy; [2]CSGI – Center for Colloid and Surface Science, Italy; [3]INSTM- Consorzio Interuniversitario per la Scienza e Tecnologia dei Materiali, Italy

This study focuses on the circular bioeconomy, aiming to valorize agricultural by-products through the extraction and encapsulation of bioactive compounds for applications in the biocosmetic field. The research develops and optimizes lipid-based nanocarrier systems, specifically liposomes and solid lipid nanoparticles, designed to enhance physicochemical stability of labile molecules, improve bioavailability, and enable controlled release[1]. Nanocarriers are produced using environmentally sustainable approaches, based on biocompatible lipids and low-toxicity surfactants, in line with green formulation principles. Comprehensive physicochemical characterization is performed using advanced analytical techniques, including Dynamic Light Scattering[2] and Nuclear Magnetic Resonance[3]. Additional investigations include complementary techniques such as Scanning and Transmission Electron Microscopy, Fourier Transform Infrared Spectroscopy, and Small Angle X-Ray Scattering. A Quality by Design strategy, supported by Design of Experiments, is applied to optimize formulation variables and ensure robustness and reproducibility. Stability of the developed lipid nanocarriers is evaluated in complex dispersing media to support sustainable cosmetic formulations while preserving functional properties of encapsulated bioactives over time. The study also investigates the influence of formulation parameters on particle size, polydispersity, surface charge, and encapsulation efficiency, which are critical for stability and performance. Particular attention is given to the selection of raw materials derived from renewable sources, ensuring alignment with circular economy principles and reduction of environmental impact. Process conditions are carefully controlled to minimize energy consumption and solvent use, reinforcing sustainability goals. The resulting nanocarriers are further assessed for their potential incorporation into cosmetic matrices, evaluating compatibility, texture, and overall product stability. This integrated approach aims to provide scalable and reproducible solutions for the cosmetic industry, promoting innovation through the use of natural resources and advanced nanotechnology. Ultimately, the research contributes to the development of high-value products from agro-industrial residues, supporting sustainability and resource efficiency in modern formulation science while addressing consumer demand for safe, effective, eco-friendly products.

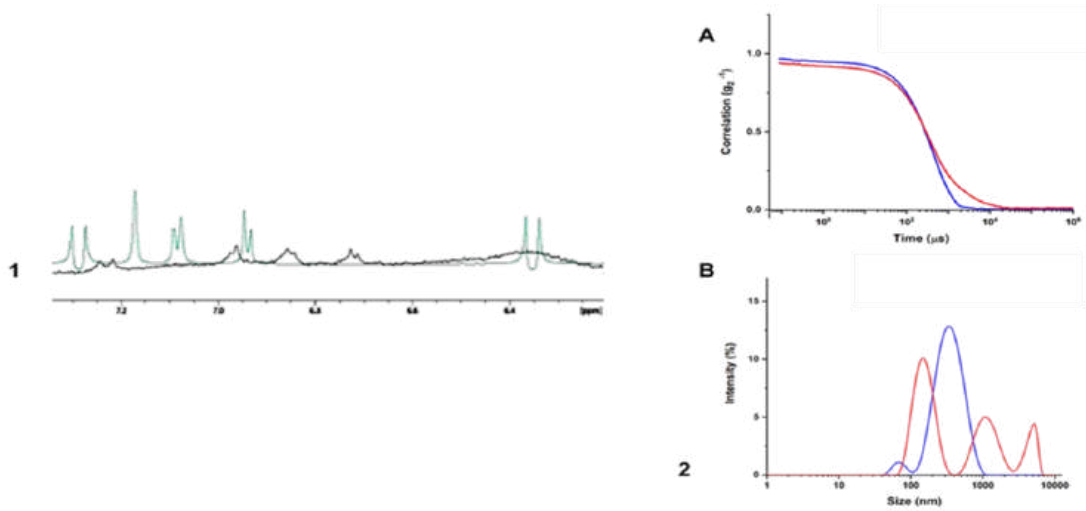

Fig. 1 [1]H NMR overlapped spectra of Caffeic Acid standard and Caffeic Acid encapsulated into DOPC-DOPE liposomes, in green and black, respectively
Fig. 2 Comparison of one-month stability between Sinapic Acid-loaded DOPC-DOPE liposomes and empty liposomes, in blue and red, respectively; Fig(2A): DLS Correlogram, Fig(2B): Intensity-based Size Distribution

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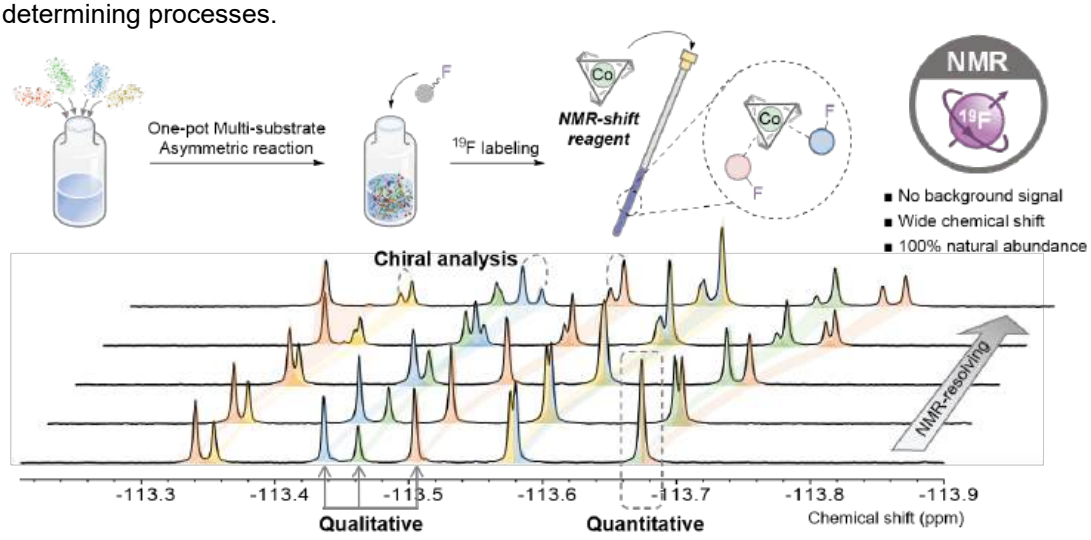
APC - D4 - P11

One-pot multisubstrate screening for asymmetric catalysis enabled by ^{19}F NMR-based simultaneous chiral analysis

Donghun Kim[1], Gyeongsun Choi[1], Hyunwoo Kim*[1]
[1]Dept. of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Korea

Exploring a diverse chemical space is essential for advancing asymmetric synthesis.[2] The complexity of the chirality-determining processes often requires resource-intensive optimization campaigns across multiple substrates.[3] Although one-pot multisubstrate screening offers a promising solution for high-throughput screening (HTS), a persistent challenge lies in the accurate and efficient analysis of complex reaction mixtures, which has traditionally relied on chromatography-based techniques with limited resolution.[4] In this work, we present a rapid multisubstrate screening workflow that utilizes ^{19}F NMR spectroscopy for simultaneous chiral analysis. By employing an NMR-shifting cobalt reagent, we accurately determined both yields and enantiomeric excesses for up to 21 different substrates in a single reaction mixture during the ruthenium-catalyzed asymmetric reductive amination of ketones. This method facilitates precise chiral analysis through dynamic peak shifts and splitting in ^{19}F NMR spectra induced by the shift reagent.[5] This approach accelerates the evaluation of structure-selectivity relationships, offering valuable mechanistic insights into enantio-determining processes.



Simultaneous analysis using 19F NMR spectroscopy and NMR-shift reagents

This work was funded by the following (to H.K.): National Research Foundation of Korea (NRF) grants RS-2023-00219859 and RS-2024-00356952; the KAIST Grand Challenge 30 project (KC30) in 2024 (N11240015).

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APC - D4 - P12

Development and validation of an LC-MS/MS method for the simultaneous determination of alprazolam, bromazepam, clonazepam, diazepam and flunitrazpam in human urine and its application to samples from suspected drug abusers

Husein Kamal [1], Varun Gandhi [1], Lina Akil [1], Naser F Al-Tannak [2], Nicholas J W Rattray [1], Ibrahim Khadra [1]
[1]Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, UK; [2]Dept. of Pharmaceutical Chemistry, Faculty of Pharmacy, Kuwait University, Kuwait

A simple and reliable method was developed using LC-MS/MS to quantify alprazolam, bromazepam, clonazepam, diazepam, and flunitrazepam in clinical samples. This method was validated for the simultaneous determination of alprazolam, bromazepam, clonazepam, diazepam, and flunitrazepam. It was applied to human urine samples collected from people suspected of drug abuse in the Kuwaiti region. Formic acid in water and acetonitrile was used in mobile phase with a gradient mode of elution using C18 reverse-phase column. The instrument was operated in a positive mode with an electrospray ionization source using multiple reaction monitoring. For sample extraction, the liquid-liquid extraction technique was used. The method was validated for limit of detection, limit of quantitation, selectivity, linearity, accuracy, and precision. The concentration for limit of quantitation was 6.0 ng/mL, the linearity ranged from 2.0 to 300 ng/mL for each of the analytes, and the r^2 values were ≥0.99. The accuracy was found to be within a range of 80-120% and precision had a %RSD of ≤15% for each of the analytes. The method was applied to 48 urine samples collected from those suspected of drug abuse by the Toxicology Dept. of the General Dept. of Criminal Evidence, Kuwait, and alprazolam, bromazepam, clonazepam, diazepam and flunitrazepam were identified commonly in the samples. The overall drug positivity rate obtained considering 48 samples was 93.75%. Based on these results and successful determination of alprazolam, bromazepam, clonazepam, diazepam and flunitrazepam in human urine samples from those suspected of drug abuse, this method is deemed to be suitable for its routine analysis.

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Posters

Computational Chemistry & AI: The Power of Data (CAI)

CAI - D1 - P01

Synergistic hydrogen-bonding and CO_2 Activation: A sustainable metal, halogen, and solvent-free strategy

Aditi Chandrasekar
Azim Premji University, India

Rapid industrialization intensifies environmental challenges by elevating atmospheric CO_2 levels, driving global warming, and ecosystem disruption. A promising approach to mitigate these adverse effects involves strategically utilizing anthropogenic CO_2 as a sustainable C1 feedstock for synthesizing cyclic carbonates, which have various industrial applications, such as electrolytes in Li-ion batteries, precursors for polycarbonates among others. Conventional catalytic methodologies for the cycloaddition of CO_2 into epoxides predominantly rely on transition metal-based catalysts in conjunction with detrimental halide-containing co-catalysts. The current research[1] endeavours to synthesize a pyrimidine-based bifunctional organocatalyst via a facile one-step Schiff-base condensation reaction. The synthesized organocatalyst efficiently transformed a wide range of epoxides into cyclic carbonates without solvents and co-catalysts. Comprehensive experimental investigations elucidated how the catalyst facilitates the reaction, emphasizing the intricate interplay of hydrogen bonding, spatial arrangement, and catalyst-substrate interactions that govern the success of this catalytic process. A meticulous analysis using density functional theory (DFT) calculations revealed that hydroxyl groups play a pivotal role in epoxide activation via hydrogen-bonding interactions, while imine nitrogen facilitates CO_2 activation through carbamate intermediate formation.

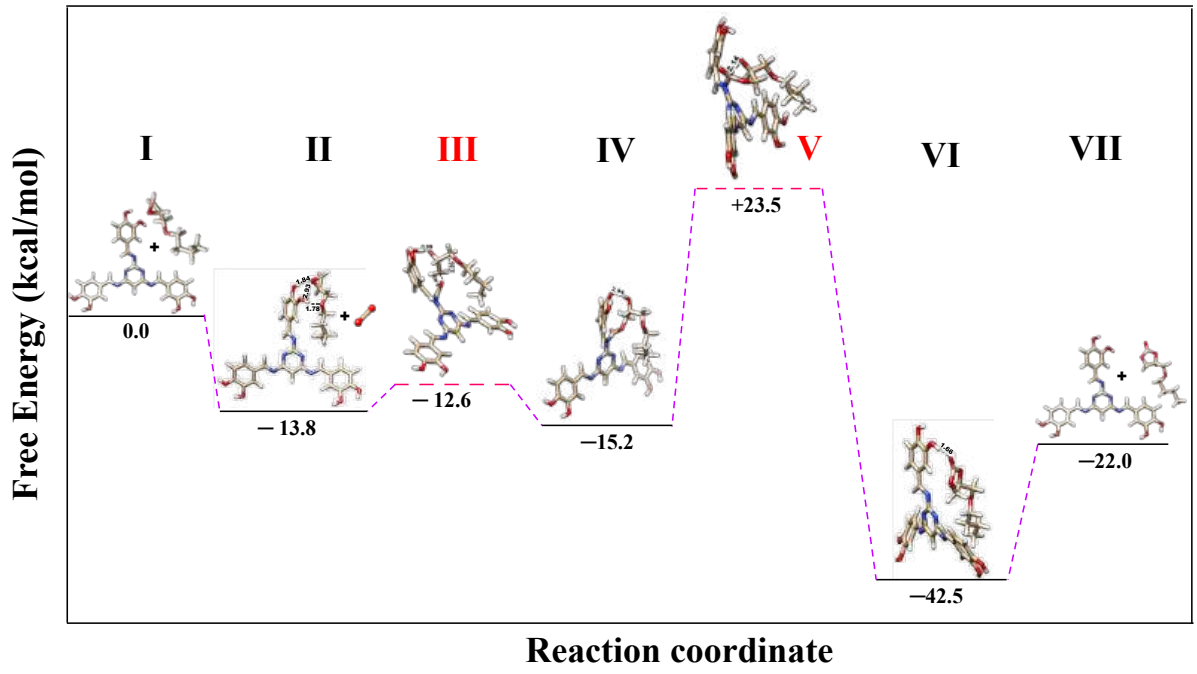

Fig. Reaction pathway along with the free energy associated with each step provided below the structure. The transition state structures are distinguished by dashed lines below them and minima geometries lie on solid lines. Interaction distances are provided in the inset.

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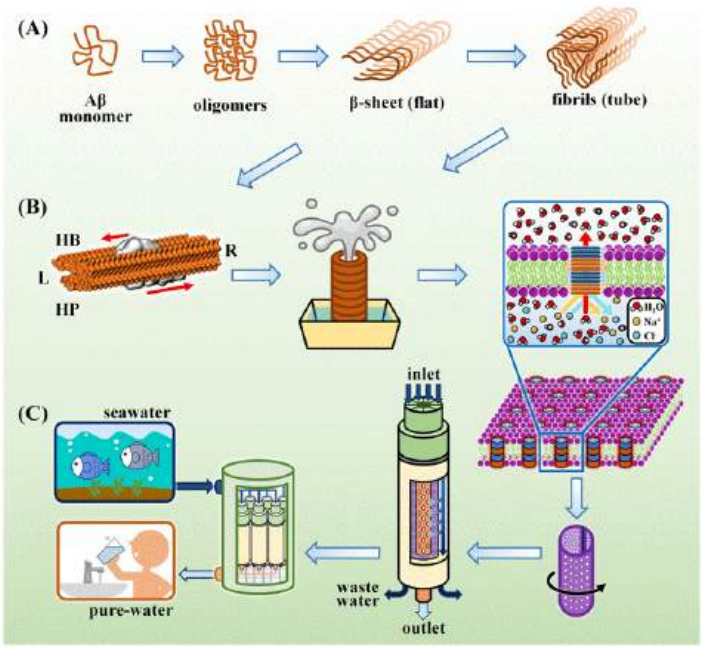
CAI - D1 - P02
High-performance energy-free desalination

Sheh-Yi Sheu[1]
[1]Dept. of Life Sciences and Institute of Genome Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan

Climate change is causing droughts and water shortages. Membrane desalination is one of the most widely employed conventional methods of creating a source of clean water, but is a very energy-intensive process. Membrane separation requires high salt selectivity across nano-channels, yet traditional techniques remain inefficient in this regard. Herein, a bioinspired, chemically robust, amyloid–fibril-based nanotube was designed, exhibiting water permeability and salt rejection properties capable of providing highly efficient desalination (Scheme 1). Molecular dynamics simulations show that nano-dewetting facilitates the unidirectional motion of water molecules on the surface of amyloid beta (Aβ) sheets owing to the ratchet structure of the underlying potential surface and the broken detailed balance. The water inside the self-assembled Aβ nanotube (ABNT) overflows, while the passage of salts can be blocked using amphiphilic peptides. The designed nanofilter ABNT shows 100% desalination efficiency with perfect NaCl rejection. The production of ≈2.5 tons of pure water per day without any energy input, which corresponds to a water flux up to 200 times higher than those of existing commercial methods, is assessed by this simulation method. These results provide a detailed fundamental understanding of potential high-performance nanotechnologies for water treatment.

Acknowledgement: The author gratefully thanks the National Science and Technology Council of Taiwan for financial support via grants NSTC (113-2113-M-A49-027, 113-2811-M-A49A-004, 114-2113-M-A49-015, and 114-2811-M-A49A-004).

ORCID:0000-0002-4416-4336



Scheme 1

[1]Liu, Y. C.; Yang, D. Y.; Deng, J. P.; Sheu, S. Y.* *Small* **2023**, 2205420.

CAI - D1 - P03
BONAFIDE: A python package for calculating features for atoms and bonds in molecules

Lukas M. Sigmund[1]
[1]AstraZeneca Gothenburg, Sweden

Molecular descriptors are essential for all cheminformatics projects, including the training of ML models. Several general software packages have been developed that facilitate the mapping between a molecular entity and a given descriptor thereby granting practitioners straightforward access to hundreds of values per molecule. While global descriptors are very important, there are many scenarios in chemistry in which local information, that is, descriptors for atoms and bonds, is indispensable. For example, the modeling of regio- and site-selectivity requires local features. In the context of medicinal chemistry, site-of-metabolization predictions or the precise description of protein-ligand interactions can be based on local atom and bond descriptors.
Several separate software tools have been developed for the calculation of specific atom and bond features. However, a consistent interface to the individual featurization tools does not exist, which hampers easy access to respective features. Therefore, we have developed the Bond and Atom Featurizer and Descriptor Extractor (BONAFIDE). It is a Python package that provides a uniform API to 11 featurization dependencies combined with from-scratch feature implementations, in total spanning 460 atom and 120 bond descriptors. Data can be obtained from SMILES strings (2D representation) as well as from XYZ or SD files (3D representations). The package ensures consistent atom and bond indexing across different data formats and facilitates processing steps such as the identification of specific functional groups or the analysis of molecular symmetry. Moreover, BONAFIDE interfaces with quantum chemistry engines to extract electronic-structure-based features; previously generated electronic structure data can also be used. Lastly, the feature output format can be widely customized, and users can implement custom featurizers in a straightforward manner. BONAFIDE includes a detailed online documentation, and the package's applicability is demonstrated with two case studies.

```
>>> from bonafide import AtomBondFeaturizer
>>> f = AtomBondFeaturizer()
>>> # Get the list of the desired feature indices
>>> fdf = f.list_features(feature_type="atom", origin="RDKit", dimensionality="2D")
>>> fidx_list = fdf.index.to_list()
>>> print(len(fidx_list))
46
>>> # Read in the molecule and calculate the features
>>> f.read_input("O=C(O)Cc1ccccc1Nc1c(Cl)cccc1Cl")
>>> f.featurize_atoms(atom_indices="all", feature_indices=fidx_list)
>>> # Get the results
>>> f.return_atom_features()
...
```

Fig. 1. *Getting started with the atom and bond featurizer BONAFIDE*: get all 2D RDKit features for all atoms in a molecule starting from a SMILES string.

CAI - D1 - P04

Predictive inorganic synthesis from small data using machine learning: Size-controlled Cu nanoparticles

Brent Motmans[1,2,3,4], Digvijay Ghogare[3,4,5,6], Thijs G.I. van Wijk[1,3], An Hardy[3,4,5], Danny E.P. Vanpoucke[1,]
[1]Hasselt University, Institute for Materials Research (imo-imomec), Quantum & Artificial inTelligence design Of Materials (QuATOMs), Belgium; [2]Hasselt University, Institute for Materials Research (imo-imomec), Hybrid Materials Design (HyMaD), Belgium; [3]imec, imo-imomec, Belgium; [4]Energyville, imo-imomec, Belgium; [5]Hasselt University, Institute for Materials Research (imo-imomec), Design and Synthesis of Inorganic Materials (DESINe), Belgium; [6]Electrochemistry Excellence Centre (ELEC), Materials & Chemistry Unit, Flemish Institute for Technological Research (VITO), Belgium

Copper nanoparticles (Cu NPs) have a broad applicability, yet their synthesis is sensitive to subtle reaction parameter variations. This sensitivity, combined with the time- and resource intensive nature of experimental optimization hinders reproducible and size-controlled synthesis. While machine learning (ML) offers a promising alternative, most approaches rely on large datasets that are rarely feasible in laboratory-scale research. Here, we demonstrate that accurate and interpretable prediction of Cu NP size is possible using a carefully curated small experimental dataset (Figure 1). A set of 25 microwave-assisted polyol syntheses was generated using Latin Hypercube Sampling to efficiently cover the parameter space defined by copper precursor concentration, reaction temperature, and time. Particle sizes were determined by dynamic light scattering, and the dataset was modeled using ensemble regression techniques implemented in the AMADEUS framework (Figure 1).[1,2] The final ensemble regression model predicts Cu NP size with a coefficient of determination of $R^2 = 0.74$ and a mean absolute error of 23.8 nm, significantly outperforming a classical design-of-experiments approach ($R^2 = 0.60$). Through systematic feature selection and regularization, the model was reduced to six physically interpretable features, improving generalization while retaining predictive accuracy. Experimental validation by synthesizing Cu NPs targeting three specific particle sizes, achieving good agreement for two out of three targets. Overall, this study highlights that, for lab-scale synthesis optimization, high-quality small datasets combined with classical, interpretable ML models outperform traditional statistical methods and are fully sufficient for quantitative synthesis prediction. This approach provides a sustainable and experimentally realistic route toward data-driven inorganic synthesis design.[3]

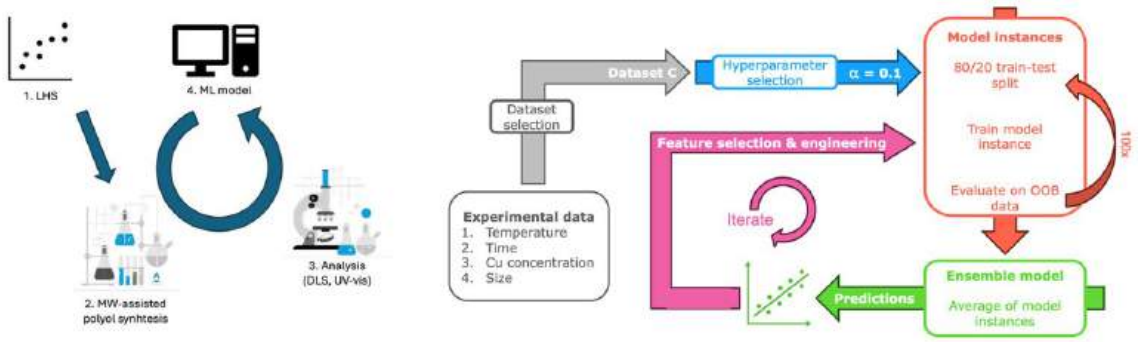


Fig. 1. Schematic representation of the synthesis workflow (left), with detailed workflow of the ML approach (right).[3]

The computational resources and services used in this work were provided by the VSC (Flemish Supercomputer Center), funded by the Research Foundation Flanders (FWO) and the Flemish Government–department WEWIS.

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CAI - D1 - P05

Defect mediated surface modification of amorphous TiO_2 surface using Grignard reagent in explicit solvation model

Krithika Ganesan[1], Erik C. Neyts[1*]
[1]*University of Antwerp, Belgium*

Titanium dioxide is extensively employed in catalysis and energy conversion due to its inherent redox stability and adaptable surface chemistry[1]. Among its various crystalline forms, the anatase polymorph demonstrates enhanced catalytic activity, However, it is the amorphousness that sometimes plays crucial roles in technical applications in sorption and separation technology which is attributed to its high surface area and electronic mobility. While conventional surface modification techniques typically rely on oxygen-based anchoring[2], organometallic functionalization, particularly through the use of Grignard reagents, offers a direct pathway to form Ti–C bond formation[3]. This approach facilitates stronger electronic coupling and enables precise tuning of interfacial properties.
We employ DFT+U simulations to examine the adsorption and reactivity of methyl magnesium bromide, coordinated by tetrahydrofuran, on amorphous TiO_2 surfaces. A key focus was understanding how both intrinsic defects[4] and the explicit dynamics of the solvent influence the thermodynamic and kinetic aspects of this surface modification process by ab-initio molecular dynamics. The results indicate that the solvent plays a crucial role in stabilizing Grignard intermediates and promoting Ti–C bond formation by enhancing Mg–C activation. Furthermore, defective sites are shown to boost charge transfer and reinforce the organometallic binding. These findings underscore the influence of solvent-mediated dynamics on Grignard reactivity and provide fundamental mechanistic insights for the directed functionalization of TiO_2 surfaces using organometallic compounds.

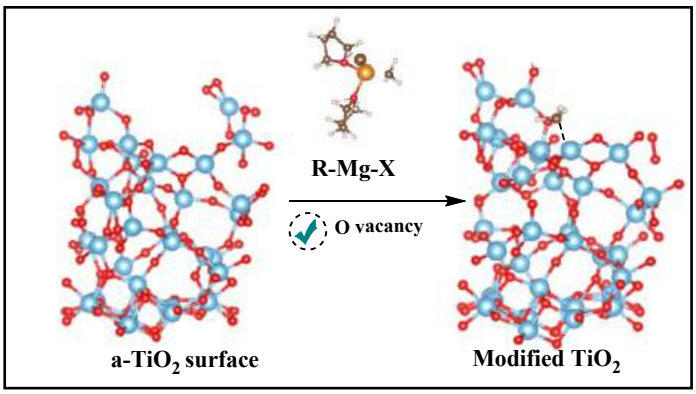

Fig. 1. Surface modification process of amorphous titania(a-TiO2) using Grignard reagent(RMgX)

The resources and services used in this work were provided by the VSC (Flemish Supercomputer Centre), funded by the Research Foundation—Flanders (FWO) and the Flemish Government.

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CAI - D1 - P06

Theoretical study of the interaction between 3α-hydroxysteroid dehydrogenase and androsterone

Kei Odai[1], Teruki Yoshimura[2], Etsuro Ito[3]
[1]Kokushikan University, Japan; [2]Health Sciences University of Hokkaido, Japan; [3]Waseda University, Japan

Introduction: 3α-hydroxysteroid dehydrogenase (3α-HSD) is an oxidoreductase that catalyzes the following chemical reaction:

Androsterone + $NAD(P)^+$ <--> 5α-Androstane-3,17-dione + NAD(P)H + H^+

It is not still unclear how 3α-HSD recognizes its ligand, androsterone. The purpose of this study is to elucidate, by using molecular dynamics and density functional calculations, how androsterone binds to 3α-HSD and how it is converted between oxidized and reduced forms. Therefore, we observed how 5α-androsterone and 5β-androsterone are incorporated into 3α-HSD using molecular dynamics simulations.

1) As a structural model of 3α-HSD, the crystal structure of human 3-alpha hydroxysteroid/dihydrodiol dehydrogenase (AKR1C4) complexed with $NADP^+$ (PDB ID 2FVL) from the Protein Data Bank was used. This 2FVL crystal structure is a trimer, containing chains A, B and C and $NADP^+$ bound to each chain. For molecular dynamics calculations, we used chain A and its associated $NADP^+$.
2) Molecular models of the ligands, 5α-androsterone (5α-ANS) and 5β-androsterone (5β-ANS), were optimized using Gaussian 09 with the density functional theory method b3lyp and the basis set 6-311++g(d,p).
3) Optimized androsterone molecule (5α-ANS or 5β-ANS) was inserted into the 3α-HSD model (2FVL (chain A) and $NADP^+$) data. The initial position of androsterone was placed outside the 3α-HSD.
4) The force fields of Amber FF14SB and GAFF2 were used. Minimization and equilibration calculations were performed using Amber 16, followed by NPT ensemble calculations.

The results showed that the recognition process differed depending on whether the ligand was 5α-ANS or 5β-ANS. We report on the structural changes of the entire 3α-HSD molecule and the structural changes of $NADP^+$ present in 3α-HSD during the process of recognizing androsterone molecule. The results suggest that 3α-HSD and $NADP^+$ undergo considerable structural changes to accommodate the ligand molecule, depending on the shape of the ligand molecule.

CAI - D1 - P07

Chemical accuracy in computational prediction of PFAS-cyclodextrin binding: A Multi-level sqm/qm study with experimental ITC validation

Christopher J. Hobbs[1], Michal Řezanka[1], Stanisław Wacławek[1]
[1]Technical University of Liberec, Institute for Nanomaterials, Advanced Technologies and Innovation, Czechia

Cyclodextrin (CD) is a naturally occurring cyclic oligosaccharide molecule which has remarkable properties owing to the hydrophobic cavity of the CD, where host-guest binding can occur, shown to bind a vast array of molecules including pharmaceuticals, water pollutants, pesticides, and more recently PFAS. PFAS, being per-/poly-fluoroalkyl substances are increasingly illustrated to be a troublesome pollutant due to their persistence, resistance, and toxicity. With remediation technologies currently inept for many of the PFAS present, CD and their derivatives have become the focus of much research as a strategy for capture of these problematic PFAS. Except for NMR titrations, which is exceptional for observing the site-specific interactions between PFAS-CD complexation, there has been no direct thermodynamic analysis of PFAS-CD complexation using calorimetry. Further, there is no computational prediction for PFAS-CD binding, likely due to, hisotrically, finding an adequate balance between computational cost and accuracy remainining a bottleneck in CD chemistry. This work presents the first systematic DFT-level investigation of PFAS-CD binding, applying Grimme's CREST/CENSO multilevel strategy to the homologous series PF4 through PF8 with native β-CD (Figure 1), wherbey we achieve chemical accuracy (MAE = 0.71 kcal mol^{-1}) against experimental ITC measurements.
Findings show that electronic energies correlate nearly perfectly with experimental total free energies. Further, chain-length selectivity is governed primairly by electronic interactions—specifically van der Waals forces and electrostatics—with solvation and entropic corrections contributing an approximately constant offset. Notably, extensive van der Waals interactions occur along the fluorocarbon backbone with anchoring by three carboxylate-to-primary-rim hydrogen bonds. Energy decomposition revealed that differential solvation penalties discriminate the binding affinity, which could explain why shorter chains, found to insert more deeply, bind more weakly because desolvation costs outweigh favorable geometry[1]. This validated workflow is robust and efficient, enabling computational screening of modified CDs and alternative PFAS structures for rational remediation system design.

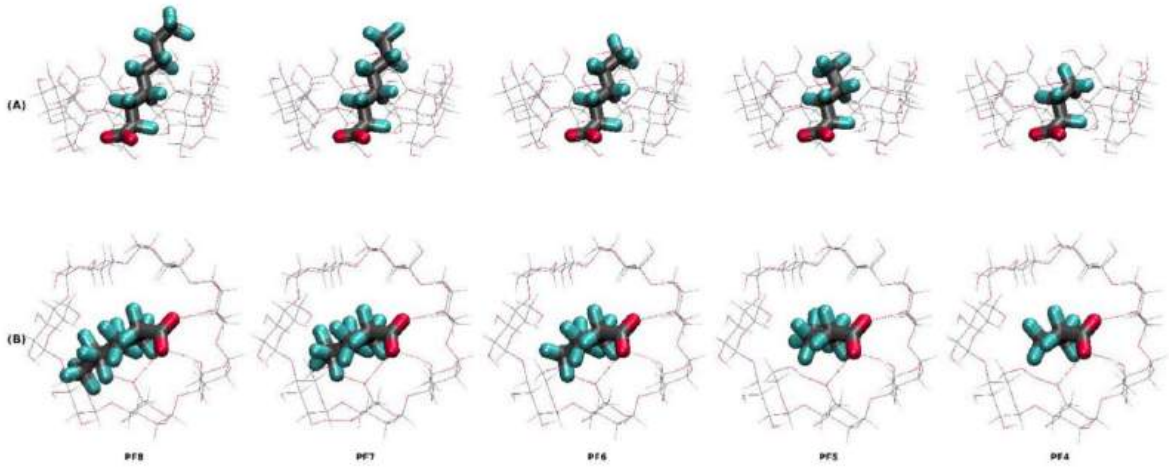

Fig. 1. Lowest-energy conformers of β-cyclodextrin complexes with perfluoroalkyl acids of varying chain length. (A) Side view; (B) top view from secondary rim, showing the H-bonding by red dashed line. PFAS: space-filling (cyan: CF_2/CF_3, red: COO^-); cyclodextrin: line representation.

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CAI - D2 - P01
Molecular quantum computer

Sheh-Yi Sheu[1]
[1]Dept. of Life Sciences and Institute of Genome Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan

Quantum computers (QCs) adopt an n-state quantum mechanical system to manipulate the superposition state. However, molecular transistors are not used to build up the quantum logic gate. Herein, it is demonstrated that DNA, RNA, and protein are promising media for QCs, and one uses residue pairs, including nucleotide base pairs and amino acid pairs, via proton-coupled electron transfer to fabricate a quantum logic gate. In the residue pair, the proton transfer between donor and acceptor states fulfills a qubit. Both the DNA-CG (3-qubit) nucleobase pair and nucleotide base pair obey the Toffoli gate. AT (2-qubit) nucleotide base pair behaves as a SWAP gate and a CNOT gate. Furthermore, the AU and RNA-CG nucleotide base pairs follow the CNOT gate and Toffoli gate, respectively. In addition, a pair of amino acids achieves 1-qubit and satisfies the Pauli-X, -Y, and -Z gates. The generators of universal quantum logic gates are obtained.

ORCID: 0000-0002-4416-4336

Acknowledgement: The author gratefully thanks the National Science and Technology Council of Taiwan for financial support via grants NSTC (113-2113-M-A49-027, 113-2811-M-A49A-004, 114-2113-M-A49-015, and 114-2811-M-A49A-004).

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CAI - D2 - P02

Towards circular design of thermoset polyurethanes: harnessing molecular dynamics and density functional theory for the depolymerization reactivity

Seppe Verheyen[1,2], Pieter Billen[3], Frank De Proft[1], Remco W.A. Havenith[2,4]
[1]ALGC, Vrije Universiteit Brussel, Belgium; [2]Molecular Energy Materials, Stratingh Institute for Chemistry and Zernike Institute for Advanced Materials, University of Groningen, The Netherlands; [3]iPRACS, University of Antwerp, Belgium; [4]Ghent Quantum Chemistry Group, Ghent University, Belgium

The circular economy for polyurethanes (PUR), a carbamate-bond containing product of multifunctional isocyanates with polyols, remains the most challenging among polymer classes, due to their complex formulation and thermoset nature hindering mechanical recycling. Both policy- and consumer-driven, PUR needs to follow industry's shift to more recycled content;[1] efficient depolymerization (Scheme 1) is imperative to reach circularity for this plastic with, on a mass basis, the largest impact on climate change.[2] However, no scaled technologies to deliver two separate streams of polyols and aromatics (from the isocyanates) are known due to PUR's complexity and side reactions.[3] Quantum-chemical modeling allows the creation of kinetic and thermodynamic data to optimize such depolymerization process design, ultimately rendering the different reaction mechanisms, barriers and interplays between them. Despite empirical knowledge, even the 3D structure of such complex PUR networks often remains elusive though, challenging a computational approach. Moreover, most molecular dynamics (MD) force fields, having been parametrized on biomolecules, are not apt to describe polymeric mixtures. Hence *ab initio* Hessian calculations are employed to enhance and tailor such force fields towards the PUR mixtures,[4] allowing physically relevant MD simulations to showcase the complex interplay of chains and solvent and the importance of noncovalent interactions (with the NCI Index) in the network.[5] With these conformations, the various possible reaction paths are elucidated with density functional theory (DFT), after a density functional benchmark. Not only granting insight in the probability of (side) reactions, it defines collective variables for use in subsequent QM/MM metadynamics, to gauge the effects under operating conditions and to retrieve the relevant rate constants for such process optimization. Opening the door for the search of new catalysts and nucleophiles, selective depolymerization and a solidified connection between theory and experiment, the depolymerization of PUR will be the foundation of industry's circular innovation.

Scheme 1. The depolymerization of polyurethane is typically carried out with a glycol nucleophile in the 'glycolysis' process. Also the 'aminolysis' is currently under investigation, using an amine such as ethanol amine as nucleophile.

S.V. thanks the Research Foundation Flanders (FWO) for the fellowship of Strategic Basic Research 1SA0226N.

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CAI - D2 - P03
Complex absorbing potentials for density functional theory

Yifan Jiang[1], Charlotte Titeca[1,2], Frank De Proft[2],Thomas-C. Jagau[1]
[1]Division of Quantum Chemistry and Physical Chemistry, KU Leuven, Leuven, Belgium; [2]Research Group of General Chemistry (ALGC), Vrije Universiteit Brussel, Brussel, Belgium

When attaching an electron to a neutral molecule, the formed anion is metastable when its energy is higher than the neutral state. Such anions are also known as electronic resonances and are subject to spontaneous decay by emission of the excess electron. Electronic resonances are beyond the reach of conventional Hermitian quantum mechanics.[1] One way to describe electronic resonances is by applying a complex absorbing potential (CAPs) to the Hamiltonian.[2] The use of CAPs results in complex energies. The real part of the energy corresponds to the energy in the conventional sense, while the imaginary part is inversely proportional to the lifetime of the temporary anion.[1]
So far, the application of CAPs has been limited to Hartree-Fock theory, post-Hartree-Fock methods, and for density functional theory (DFT), the local density approximation.[3] We present the implementation of CAPs for generalized gradient approximation (GGA) functionals as well as hybrid functionals that comprise only GGA and LDA functionals.[4,5] Our implementation enables the study of temporary anions of larger molecules in a fast and accurate way. We present benchmarks testing the performance of different functionals and basis sets on various well characterized temporary anions, including those of nitrogen, formaldehyde, formic acid and ethene against equation-of-motion coupled-cluster singles and doubles (EOM-CCSD) theory. In addition, we present results for different anionic states of pyrene, a molecule too big for a CAP-EOM-CCSD treatment.

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CAI - D2 - P04
Accurate property data for small molecules from theory

Dirk Andrae[1]
[1]*Freie Universität Berlin, Germany*

Property data for isolated small molecules in their electronic ground state, like molecular structure or fundamental frequencies, are highly important in many branches of science, e. g. astrochemistry, atmospheric chemistry, heterogeneous catalysis, matrix isolation vibrational spectroscopy under cryogenic conditions, to name just a few. But the "power of data" is misled if the data is of inferior quality. As is well known, calculated property data compare very well with experimental data (see, e. g., refs. 1, 2 and references therein), if (i) the system under study – the molecule in a given electronic state – is composed of only few and light atoms (say, $Z < 10$) and if (ii) the calculated property data derive from a sufficiently high level of quantum chemical theory (typically from an explicitly correlated method like CCSD(T)-F12). This contribution shows that property data for many small molecules containing heavier atoms (up to, say, $Z = 80$ [Hg]) can be accurately calculated with a valence-only treatment.

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CAI - D2 - P05

Dissociative electron attachment to building blocks of DNA studied by *ab-initio* molecular dynamics with complex absorbing potentials

Tobias Wittemann[1], Hà-Quyen Nguyen[1], Charlotte Titeca[1,2], Thomas-C. Jagau[1]
[1]KU Leuven, Belgium; [2]Technical University of Denmark, Denmark

Ionizing radiation can induce strand breaking in DNA, leading to cell death or mutations that may cause tumors. The targeted treatment of malignant tumors with ionizing radiation, however, has proven highly successful in cancer therapy and is an established tool in modern radiomedicine. Therefore, studying the impact of ionizing radiation on DNA is essential for understanding radiation-induced damage and advancing the controlled application of ionizing radiation in cancer therapy.

It has been shown that DNA damage does not arise directly from the interaction with the primary radiation, but rather from the attachment of secondary electrons produced by ionizing radiation.[1] When such an electron attaches to a molecule (e.g. a DNA strand), the resulting anion is often temporary and may either undergo dissociation or autodetachment. A distinctive feature of dissociative electron attachment (DEA) is that electrons with kinetic energies below the bond dissociation energy can still induce bond cleavage.

In this work, we investigate DEA to DNA building blocks using *ab-initio* molecular dynamics (AIMD). However, temporary anions (TAs) pose a challenge to standard quantum chemistry methods as they are metastable electronic states embedded in the continuum and thus cannot be obtained as stationary solutions of the Schrödinger equation with a hermitian Hamiltonian. An elegant solution to this problem is provided by non-hermitian quantum chemistry, enabling the use of methods implemented in conventional quantum chemistry codes.[2] In our study, we employ a complex absorbing potential (CAP) to treat TAs. The CAP–AIMD approach allows for the simulation of the dynamics of TAs and has proven successful at describing DEA in previous work.[3]

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CAI - D2 - P06

Weak global correlations, hidden local trends: Regime-aware analysis of biochar synthesis–property data

Adriano Silva[1], Fernanda F. Roman[1], Helder T. Gomes[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Bragança, Portugal

Biochar synthesis is often guided by empirical optimization, despite the growing number of studies reporting preparation conditions and material properties. In practice, however, the information is fragmented across different parameters (*e.g.* thermal treatments, atmospheres, residence times, and characterizations). This heterogeneity makes it difficult to identify general synthesis–property relationships using conventional global analysis. In this work, a curated literature-derived dataset of biochar materials was explored to assess how synthesis descriptors relate to specific surface area. The first stage consisted of a global correlation analysis between selected preparation or composition variables and S_{BET}. The results showed that most descriptors display weak or moderate linear relationships when the full dataset is considered together. Final temperature presented a clearer association than heating rate, while compositional indicators linked to carbonization severity showed stronger correlations, as shown in Figure 1a. Nevertheless, these global trends remain limited because they merge materials prepared from different biomass sources and under different processing windows. To address this limitation, a regime-aware analysis was applied by dividing selected descriptors into defined ranges and evaluating local relationships within each subset. This approach revealed that the effect of synthesis temperature is not constant across the dataset. Instead, stronger relationships emerge only within specific regions, while other ranges show weaker or inconsistent behavior. Therefore, weak global correlations should not be interpreted as the absence of relevant synthesis effects, but as evidence that different regimes may follow different patterns. This communication highlights the importance of treating literature datasets as heterogeneous experimental spaces rather than uniform populations. By combining careful data curation with local statistical exploration, it becomes possible to uncover hidden structures [1]. Such analysis can support more interpretable machine learning strategies for biochar and other carbon materials.

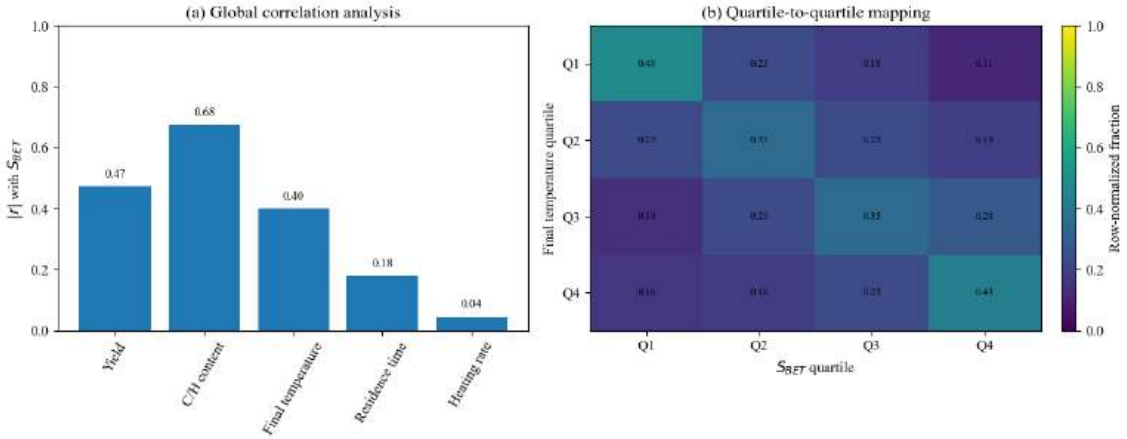

Fig. 1. (a) Global correlation coefficients (|r|) between S_{BET} and selected synthesis parameters and (b) quartile-based mapping of local correlations between final temperature and S_{BET}.

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO UID/00690/2025 (10.54499/UID/00690/2025) and UID/PRR/00690/2025 (10.54499/UID/PRR/00690/2025); SusTEC, LA/P/0007/2020 (10.54499/LA/P/0007/2020). This work was also supported by the project “3D-CARB4E&E – 3D-printed carbon monoliths for energy and environmental applications” (10.54499/2023.18105.ICDT), funded by Programa Inovação e Transição Digital (COMPETE 2030), FCT, I.P., and FEDER, and by ML3DCARB (10.54499/2024.17845.PEX).

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CAI - D3- P01

Design, synthesis and biological activity of 2AMINO5,4-B thiazolopyridine EGFR based anti-cancer agent

Mohd Aatif Shaikh
Jamia Hamdard University

The epidermal growth factor receptor (EGFR) plays a central role in tumor development and remains a validated target for anticancer drug discovery. This study demonstrates the integration of computational chemistry and data-driven approaches for the rational design, synthesis, and evaluation of novel 2-amino-5,4-b thiazolopyridine derivatives as potential EGFR-targeted anticancer agents. A library of candidate molecules was rationally designed based on EGFR pharmacophore features and synthesized through a multistep pathway. Structural confirmation was achieved using FT-IR, ^{1}H NMR, and ^{13}C NMR spectroscopy.

Molecular docking simulations were performed against the EGFR tyrosine kinase domain to assess binding affinity and key ligand–receptor interactions. Compounds exhibited favorable docking scores with significant hydrogen bonding and hydrophobic interactions within the ATP-binding pocket, suggesting strong potential for EGFR inhibition. In addition, in silico ADMET and drug-likeness predictions using data-driven tools supported favorable pharmacokinetic properties and compliance with Lipinski's rule of five, indicating drug-like characteristics.

The integration of computational modeling and predictive analytics significantly accelerated lead prioritization and reduced experimental optimization cycles. These results highlight the promising role of computational chemistry and AI-assisted data analysis in guiding the discovery of new EGFR-focused anticancer agents, warranting further biological evaluation.

CAI - D3- P02
From manual operation to autonomous STM via visual reasoning AI

Shaoxuan[1], Steven De Feyter[1]
[1]Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Belgium

Scanning Tunnelling Microscopy (STM) is an indispensable tool in surface science and physical chemistry. For instance, this local probe microscopy technique not only allows for the visualization of molecular patterns, monolayer-thin covalent organic frameworks and metal organic frameworks, but also their growth dynamics, with submolecular resolution [1-3]. Yet its operation remains largely manual, time-intensive, and dependent on expert intuition. While many STM systems are built on legacy digital infrastructures, recent access to instrument-level application programming interfaces (APIs) enables new opportunities for advanced automation beyond conventional scripting.

Here, we present a Brain–Puppet hierarchical AI architecture for autonomous STM operation that integrates multimodal visual language models (VLMs) with direct instrument control. A modern external computer hosts a VLM acting as a virtual scientist, which continuously interprets real-time STM images and graphical interface feedback. This enables semantic understanding of experimental states, such as distinguishing molecular features from noise, diagnosing unstable tunnelling conditions, and identifying atomically flat terraces suitable for high-resolution imaging.

High-level experimental strategies generated by the VLM are translated into structured control commands and executed through the STM's native APIs. This hierarchical separation preserves both intelligence and safety, experiment-level reasoning is handled by the AI agent, while the STM's internal feedback loops and PID controllers maintain atomic-scale stability.

By combining visual semantic understanding with instrument-level control, this approach enables adaptive and context-aware experimentation and represents a practical step toward self-driving laboratories in surface chemistry.

Acknowledgements: Financial support from KU Leuven–Internal Funds (C14/23/090), FWO (I006922N), and Chinese Scholarship Council (grant No.202506890042) is acknowledged.

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CAI - D3- P03

Novel antimicrobial agents: From synthetic design to integrated *in vitro* and *in silico* insights

Abrar Hussain[1,2], Sang Hyun Park [1,2]

[1]Advanced Radiation Technology Institute (ARTI), Korea Atomic Energy Research Institute, Jeongeup, Republic of Korea; [2]Radiation Science, University of Science and Technology, Daejeon, Republic of Korea

Antimicrobial resistance (AMR) has emerged as a critical global health challenge driven by the increasing prevalence of multidrug-resistant bacteria, including *Staphylococcus aureus* and *Pseudomonas aeruginosa*, as well as pathogenic fungi such as *Candida albicans* and *C. parapsilosis*. In this study, six newly synthesized Schiff base derivatives (HSB-1 to HSB-6) were systematically evaluated through an integrated experimental and computational approach to identify promising antimicrobial candidates. In vitro antimicrobial screening using disk diffusion assays revealed notable antibacterial activity against *S. aureus*, particularly for HSB-6 and HSB-1 (15–17 mm inhibition zones), while HSB-5 and HSB-6 exhibited measurable activity against *P. aeruginosa* (12 mm). Moderate antifungal effects were observed for HSB-4 against *Candida* species. To rationalize these experimental trends at the molecular level, in silico investigations were performed using molecular docking, molecular dynamics (MD) simulations, density functional theory (DFT), and ADMET profiling. Docking studies demonstrated strong binding affinity of HSB-5 toward the LasR protein of *P. aeruginosa* ($\Delta G = -12.3$ kcal mol^{-1}), supported by favorable hydrogen bonding and hydrophobic interactions. The stability of the protein–ligand complexes was further confirmed by 100 ns MD simulations, showing low RMSD values, compact radius of gyration, and persistent intermolecular interactions. DFT calculations at the B3LYP/6-311G(d,p) level provided electronic descriptors consistent with biological performance, revealing lower HOMO–LUMO energy gaps for HSB-6 and HSB-1 and an intermediate gap for HSB-5. NBO and Fukui analyses identified key electrophilic and nucleophilic sites involved in molecular recognition. ADMET predictions indicated acceptable drug-likeness for most derivatives, including favorable gastrointestinal absorption and physicochemical properties, while highlighting potential safety concerns for selected compounds. Overall, HSB-5 emerged as a balanced lead compound, combining effective in vitro antimicrobial activity with robust computational support, warranting further optimization in the fight against antimicrobial resistance.

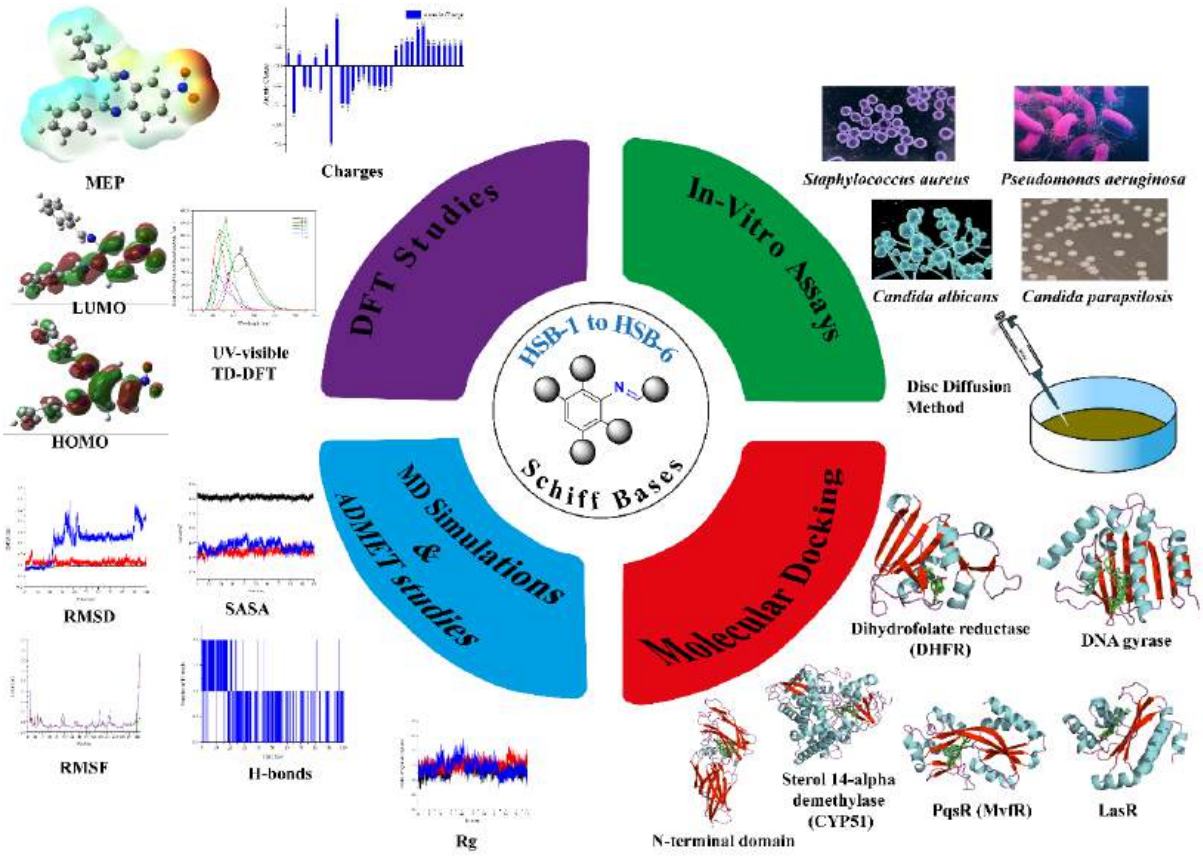

Fig. 1. Diagrammatic illustration of the synthesis of Schiff bases, their antimicrobial activity, and computational evaluation via molecular docking, MD simulations, ADMET, and DFT analysis

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CAI - D3- P04

Data-driven process optimization for selective magnesium recovery from desalination brine

Jamilu Usman[1], Qazi Iqra Shafi[2], Billel Salhi[1], Nadeem Baig[1], Dahiru U. Lawal[1,3], Sani. I. Abba[4], A.G. Usman[5], Isam H. Aljundi[1,2]

[1]Interdisciplinary Research Centre for Membrane and Water Security, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Dept. of Chemical Engineering, King Fahd University of Petroleum and Minerals, Saudi Arabia; [3]Mechanical Engineering Dept., King Fahd University of Petroleum & Minerals, Saudi Arabia; [4]Dept. of Civil Engineering, Prince Mohammad Bin Fahd University, Saudi Arabia; [5]Dept. of Analytical Chemistry, Faculty of Pharmacy, Near East University, TRNC, Turkey

The sustainable management of desalination brine is increasingly recognized as a critical pathway for both environmental protection and strategic resource recovery. This study presents an integrated experimental–computational framework for the selective recovery of magnesium from real reverse osmosis (RO) reject brine through controlled alkaline precipitation coupled with advanced machine-learning modeling. Magnesium hydroxide ($Mg(OH)_2$) was precipitated using ammonium hydroxide under systematically varied pH (10.0–11.0), temperature (15–35 °C), and initial magnesium concentrations (2100–3148.5 ppm) to delineate the operational recovery window under realistic brine chemistry. Experimental results demonstrate that pH is the dominant governing parameter for magnesium recovery, while temperature exerts a secondary kinetic influence. Under optimized conditions (pH 11, 35 °C, Mg = 3148.5 ppm), magnesium recovery reached 96.91% with a product purity of 97.05%, as confirmed by comprehensive physicochemical characterization (XRD, XRF, SEM–EDS, and TGA). To enable predictive control and operational scalability, Gaussian Process Regression (GPR), Bagged Trees (BT), and Artificial Neural Network (ANN) models were developed and refined using Bayesian Optimization. Among all models, ANN exhibited superior generalization performance on unseen data (R^2 = 0.9967, RMSE = 0.1184), accurately capturing nonlinear interactions between process variables and recovery efficiency. Principal Component Analysis further identified alkalinity control as the primary driver of recovery performance, reinforcing the experimental findings. The proposed framework bridges real-brine experimentation with data-driven intelligence, enabling accurate forecasting, informed set-point selection, and minimized co-precipitation risk. This work establishes a replicable, decision-oriented strategy for intelligent brine valorization that supports circular economy principles and advances sustainable mineral recovery in desalination systems.

This work was supported by the Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum and Minerals [Grant number INMW2511].

CAI - D3- P05
Unravelling aspartame-induced activation pathways in the TAS1R2/TAS1R3 receptor

Judith Millan and Rodrigo Martínez
Universidad de La Rioja, Spain

This work centres on the molecular dynamics simulation of a complete model of the human sweet-taste receptor TAS1R2/TAS1R3 bound to the sweetener aspartame. The system has been carefully built to reproduce a realistic biological environment. It includes the full receptor heterodimer embedded in a heterogeneous, asymmetric lipid bilayer mimicking a human cell membrane, fully solvated with explicit water and neutralising ions.
The starting structure is based on a homology-modelled human apo receptor, generated from a chimeric TAS1R2/TAS1R3.[1] Receptor's protonation state and aspartame docking on its binding site were performed by the AI assistant Playmolecule Viewer.[2]
After this, CHARMM-GUI Membrane Builder module[3] was used to insert the complex through a lipidic bilayer of made of POPC phospholipids. The final prepared system consists of around 400,000 atoms and uses CHARMM36m force-field parameters for proteins and lipids, together with CGenFF parameters for the ligand. After geometry preparation, energy minimisation and a multi-step restrained equilibration were carried out, producing a stable, simulation-ready system.
After 500 ns of NPT molecular dynamics simulations several analyses have been performed, such as hydrogen bonds identification, aspartame's, solvent accessible surface area (SASA) or principal component analysis (PCA), to characterise how ligand binding triggers structural changes across the receptor. Domain closure motions or transmitted rearrangements have been investigated to shed light into the sweet taste signal transmission.

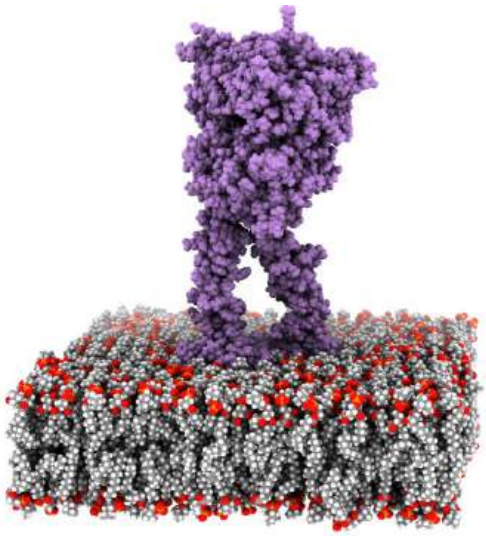

Fig. 1. TAS1R2/TAS1R3 sweet taste receptor inserted in a model lipidic bilayer

Authors acknowledge to "Ministerio de Ciencia, Innovación y Universidades del Gobierno de España" for funding through PID2021-127918NB-I00 project, SGIKER service (UPV/EHU, MICIU-FEDER) for assisting in the computational calculations, and Universidad de La Rioja for its support.

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CAI - D3- P06

Quantum computers for molecular inverse design: The quantum ensemble variational optimization algorithm

Francesco Calcagno[1,2], Delmar G.A. Cabral[3], Ivan Rivalta[1,2], Victor S. Batista[3,4]
[1]University of Bologna, Italy; [2]Center for Chemical Catalysis, Italy; [3]Yale University, USA; [4]Yale Quantum Institute, USA

Molecular inverse design is a long-standing challenge in Chemistry with the potential to dramatically accelerate the discovery of novel compounds featuring desired properties.[1] In the past decade, machine learning (ML) and artificial intelligence techniques have gained attention as cutting-edge methods to accelerate screening and generation of functional molecules.[1,2] However, ML models usually rely on large training sets, which may limit unbiased exploration of the chemical space.

Quantum computers natively implement the quantum superposition principle and offer new opportunities for fast exploration of large combinatorial spaces.[3] In the present contribution, we present the Quantum Ensemble Variational Optimization (QEVO) algorithm,[4] a variational quantum algorithm for molecular design. QEVO encodes molecules as Pauli strings using a parametrized quantum circuit. The algorithm iteratively samples ensembles of molecules, whose properties are used to improve the generation by variationally optimizing circuit's parameters (Figure 1).

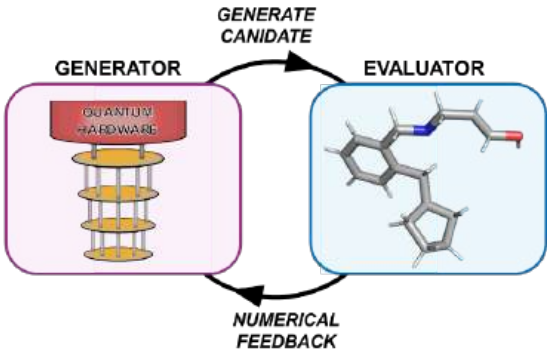

Fig. 1. Workflow of the Quantum Ensemble Variational Optimization (QEVO) algorithm.

We successfully tested QEVO in several molecular design problems with combinatorial complexity up to 2^{160} possible solutions, showing that QEVO correctly samples high-rewarding molecules despite a limited exploration of the total space.[4] Notably, QEVO was able to generate drug-like molecules with anticancer properties, highlighting its potential to pave the way towards new strategies for inverse molecular design using quantum hardware.

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CAI - D3- P08
Automated classification and quantification of pickering emulsion droplets using YOLOv7

Adriano Silva[1], João Mendes[2], Adjel Soares[2], Fernanda F. Roman[1], Ana I. Pereira[2], Helder T. Gomes[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal; [2]Research Centre in Digitalization and Intelligent Robotics (CeDRI), Instituto Politécnico de Bragança, Portugal

This work presents a deep learning-based strategy for the automatic classification and quantification of Pickering emulsion droplets using the YOLOv7 object detection tool. In complex systems such as Pickering emulsions, the presence of solid stabilizing particles complicates automated detection using conventional image-processing methods [1]. Pickering emulsions stabilized with carbon nanotubes were prepared and imaged by optical microscopy. A curated dataset of micrographs was used to train and validate two YOLO architectures (v4 and v7), with YOLOv7 demonstrating superior performance, particularly in images containing high number of small droplets. The trained model enabled rapid and reliable droplet detection, reducing analysis time from hours to seconds. Following detection, two independent quantification strategies were implemented. The first method estimated droplet diameter directly from bounding box dimensions, while the second applied a segmentation-based approach to more accurately determine droplet boundaries. The full analysis workflow is schematically illustrated in Figure 1. Comparison with manual measurements revealed that the second method achieved a mean error of only 2.74%, corresponding to an overall accuracy of 97.26%. Droplet size distributions confirmed strong agreement between automated and manual measurements, demonstrating that the coupled YOLOv7–segmentation workflow reliably reproduces both average droplet sizes and full distribution profiles, in line with recent deep-learning approaches applied to Pickering emulsions [2]. This study demonstrates the feasibility of applying deep learning tools to complex colloidal systems and highlights their potential to accelerate data extraction from microscopy images. The methodology is transferable to other emulsions and paves the way toward automated characterization platforms.

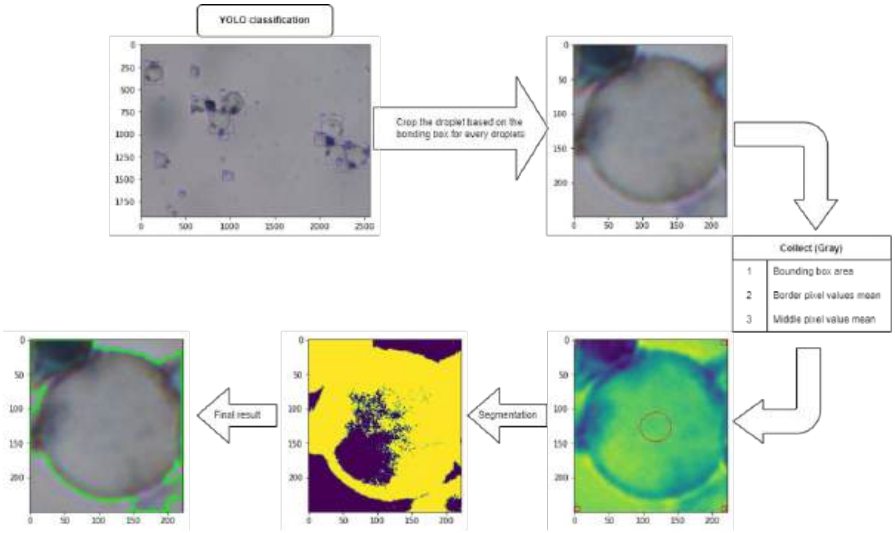

Fig. 1. Second method architecture.

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO UID/00690/2025 (10.54499/UID/00690/2025) and UID/PRR/00690/2025 (10.54499/UID/PRR/00690/2025); SusTEC, LA/P/0007/2020 (10.54499/LA/P/0007/2020). This work was also supported by the project “3D-CARB4E&E – 3D-printed carbon monoliths for energy and environmental applications” (10.54499/2023.18105.ICDT), funded by Programa Inovação e Transição Digital (COMPETE 2030), FCT, I.P., and FEDER, and by ML3DCARB (10.54499/2024.17845.PEX).

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CAI - D3- P09

A reproducible multi-scale computational workflow for DL-methionine in breast cancer targets: DFT, data-driven docking, MD and MM-PBSA validation

Md Wasee Murtuza[1], Mohd. Zaid[1], Manoj Sharma[1], Saleem Javed[1]
[1]Jamia Millia Islamia, India

The structural, vibrational, electronic and biological relevance of DL-Methionine (DL-MT), a possible anti-breast cancer agent, were explored by combining experimental FT-IR and UV-Vis spectra with density functional theory (DFT), molecular docking, molecular dynamics (MD) simulations and MM-PBSA binding free-energy estimation. For optimised geometries, harmonic vibrational wavenumbers were computed at the B3LYP/6–311++G(d,p) level, and vibrational spectrum assignments were obtained through normal coordinate analysis in conjunction with Pulay's SQMFF methodology, enabling a precise correlation between simulated and experimental spectral profiles. A comparison of DL-MT frontier molecular orbital (FMO) gaps in dissimilar environments disclosed energy gap values of 5.608 eV (gas), 5.586 eV (water), 5.577 eV (methanol) and 5.581 eV (DMSO), indicating solvent-dependent modulation of reactivity. To predict electrophilic and nucleophilic reactive sites, molecular electrostatic potential (MEP) visualisations were generated in both gas and solvent phases, and Fukui function descriptors were also assessed. Furthermore, AIM, RDG/NCI, DORI, ELF and LOL topological analyses were executed to obtain additional insight into intramolecular stabilisation and electron density localisation behaviour.
In a bid to prioritise biologically relevant targets, molecular docking was conducted against four breast cancer proteins (PDB IDs: 5NWH, 5NQR, 7ULV and 6SZQ), resulting in binding energies of -5.96, -4.51, -4.89 and -4.27 kcal/mol, respectively, and the associated interaction profiles were comprehensively examined. Specifically, 100 ns all-atom MD simulations were performed for the DL-MT complexes of 5NWH and 7ULV (highest docking affinities), and the gmx_MMPBSA protocol was utilised on MD trajectories to determine ΔG_binding values of -20.95 kcal/mol (5NWH) and -0.58 kcal/mol (7ULV). Finally, ADMET predictions and drug-likeness assessments (Lipinski compliance; HIA ≈ 81.6%; logP ~0.15) supported favourable pharmacokinetic behaviour with low predicted toxicity, suggesting DL-MT as a plausible candidate scaffold for follow-up validation[1].

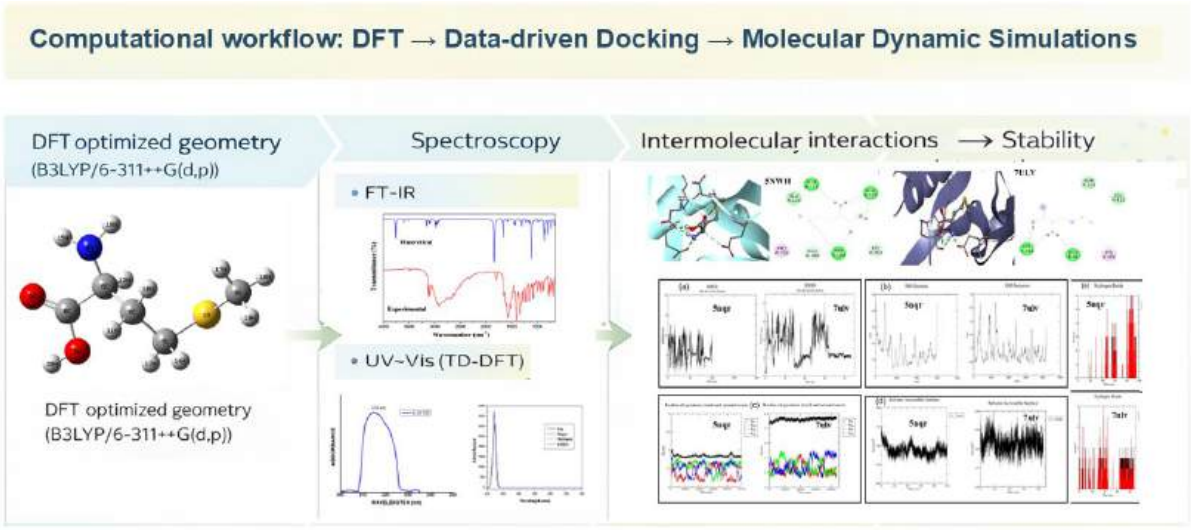

Fig. 2. Computational workflow: DFT, data-driven docking, MD.

Acknowledgement: The original study acknowledges Jamia Millia Islamia (India).

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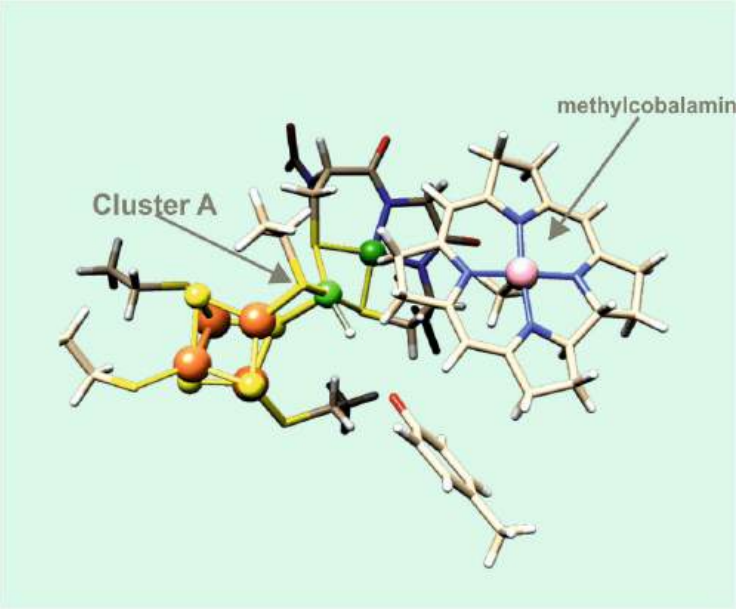
CAI - D3- P10

Mechanism of methylation of A-cluster in coenzyme A synthase by cobalamin. Insight from DFT calculations

Maria Jaworska, Piotr Lodowski
University of Silesia in Katowice, Poland

Acetyl coenzyme A synthase (ACS) catalyzes the synthesis of the acetyl group from the methyl group and carbon monoxide, ultimately leading to the formation of acetyl coenzyme A. The first step in this reaction is the methylation of the nickel ion in the A-cluster of the ACS enzyme. A-Cluster consists of a dinuclear nickel complex linked to iron-sulfur cubane, Fe_4S_4. We propose a mechanism in which the nickel atom on which the reaction occurs, is protonated in the enzyme resting state. When the methylating agent, methylcobalamin, approaches the A-cluster, the proton is transferred to a strong base. We suggest this to be the tyrosine anion, replaced in the calculations by a phenolate anion. To determine the reaction energy, the potential energy surface (PES) was calculated using the DFT/BP86 method. **The potential energy surface** was determined based on the position of the proton and the distance of methylcobalamin from the A-cluster. Calculations were also performed for the same reaction in the presence of a water molecule. The water molecule participating in the reaction facilitates proton transfer and lowers the reaction barrier.



Model of the protonated A-cluster in the presence of methylcobalamin

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CAI - D4 - P01
Model order reduction of CFD model for membrane distillation

Leon Žagar[1], Andraž Pavlišič[1], Blaž Likozar[1]
[1]National Institute of Chemistry, Slovenia

Membrane distillation (MD) is an emerging process for purifying water solutions using low grade heat such as waste heat or solar thermal energy. Optimization of membrane distillation is critical for optimal production and its viability for industrial use. Theoretical approaches such as numerical modeling of chemical processes can predict the system behavior and inhibited performance such as lower mass flux due to concentration and temperature polarization. Simulations can give insight to processes and provide data of hard to measure properties such as membrane surface temperature. Computational fluid dynamics (CFD) simulation is widely accepted as a tool for process simulations. The complex setup of CFD and high computational cost are needed for a simulation. To decrease the high computational cost, a model order reduction numerical simulation and machine learning (ML) model were made to calculate the mass flux through the membrane region. A direct-contact MD module process was simulated using CFD and model order reduction in-house Python code was created to simulate the temperature inside the MD module. The reduced-order model was validated against CFD and experimental data, indicating similar performance in predicting the mass flux. A trained neural network provided a data-driven prediction method for mass flux in a DCMD module. The results show that model order reduction and data-driven approaches can predict the mass flux with high prediction accuracy, offering simpler performance prediction with a lower computational cost.

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CAI - D4 – P02

Cross-validated screening of natural products targeting two distinct functional sites of the bacterial ribosome: An in-silico study

Nesrin Isil Yasar[1], Fethiye Aylin Sungur[1], Ozge Kurkcuoglu[2]

[1]Computational Science and Engineering Division, Informatics Institute, Istanbul Technical University, Istanbul, Türkiye; [2]Dept. of Chemical Engineering, Istanbul Technical University, Istanbul, Türkiye

The World Health Organization identifies antibiotic resistance as a critical global health threat, necessitating the development of novel therapeutic strategies [1]. The bacterial ribosome is one of the primary targets for antibiotic development due to its vital role in protein synthesis, specifically within the decoding center (DC) and peptidyl-transferase center (PTC) [2]. Natural products represent superior alternatives to traditional synthetic libraries, as they possess higher sp^3 carbon content, richer hydrogen bonding profiles, and lower toxicity risks [3]. This study explores natural product candidates targeting DC and PTC regions of the *E. coli* ribosome. In this research, an integrated collection of natural product libraries was screened against these ribosomal sites. The computational workflow was validated through redocking crystallographic ligands using Glide [4] and AutoDock Vina [5]. Following docking, binding affinities were refined using Prime MM-GBSA. To prioritize candidates, refined hits underwent rigorous filtering, including substructure analysis, ADME property evaluation, and fingerprint-based clustering to ensure chemical diversity and drug-likeness. Structural behavior was evaluated through three independent 100 ns replica MD simulations, where trajectories were analyzed to assess molecular interaction persistence and binding free energies. This multilayered approach identified promising natural products with high affinity and stability, establishing a robust discovery workflow.

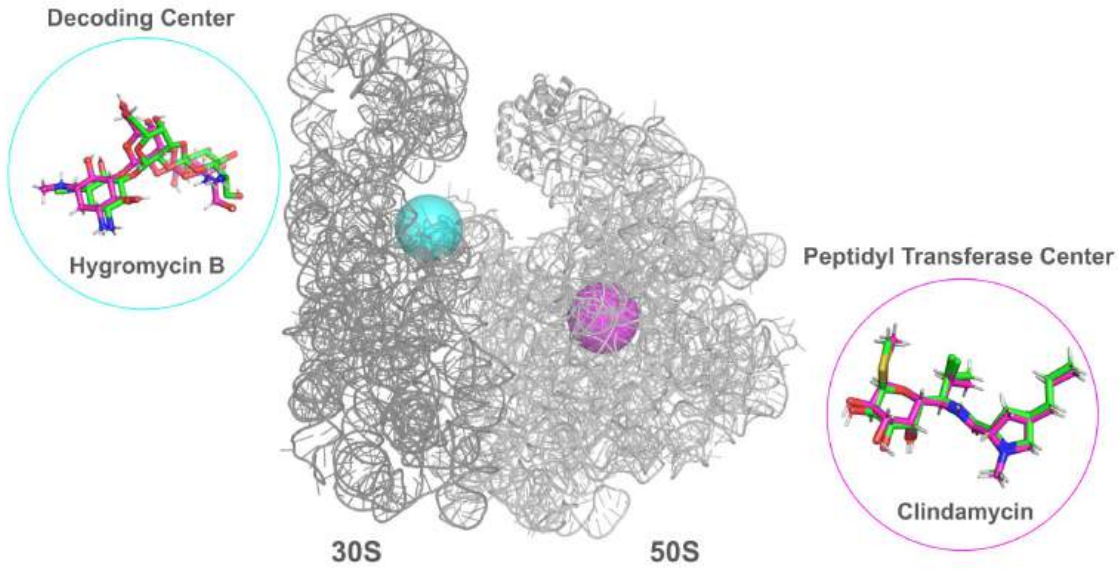

Fig. 1. 3D structure of *E.coli* 70S ribosome (crystal pose: green, best docking pose: magenta).

Acknowledgement: This work was supported by TUBITAK 1001 The Scientific and Technological Research Projects Funding Program (Project no: 121Z330).

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CAI - D4 - P03

Beyond bulk aggregation: Interfacial chloride recognition by triazolophane on graphene

Francisca Salas-Sepúlveda[1], Ricardo A. Zamora[1], Horacio Poblete[1]

[1]Dept. de Bioinformática, Centro de Bioinformática, Simulación y Modelado (CBSM), Facultad de Ingeniería, Universidad de Talca, Campus Talca, Chile

Anion recognition and capture are central to sensing, separation, and remediation, yet they remain difficult in water because hydration and receptor aggregation often suppress binding. Triazolophanes provide a useful model for this problem because their rigid frameworks and polarized C–H groups support anion recognition while remaining structurally tunable. Here, we combined atomistic molecular dynamics simulations and free-energy calculations to investigate how solvent environment and surface confinement affect chloride capture by triazolophane macrocycles, including both the parent host and an alkyl-substituted derivative, in water and organic solvents, both in bulk solution and at a graphene interface.

Comparison of the parent triazolophane with its alkyl-substituted derivative shows that hydrophobic substitution has only a limited effect in bulk solution but becomes more important at the interface, where the modified receptor adsorbs more strongly on graphene and forms more stable interfacial assemblies. Solvent then emerges as a second key factor: as the number of macrocycles increases, it strongly influences the access to the macrocycle cavity and the extent of supramolecular self-assembly. In water, hydrophobic aggregation limited chloride binding efficiency, whereas in organic solvents, the receptor cavity remains more accessible to the anion. At the graphene interface, however, this tendency changes, making chloride capture more favorable.

Overall, these results highlight interfacial confinement as a useful element in the design of surface-assisted anion-capture systems and provide a basis for developing responsive supramolecular materials for aqueous ion recognition.

Acknowledgements: R.A.Z thanks the FONDECYT grant 1240759. H.P thanks the FONDECYT grant 1251288. F.S-S. thanks ANID Ph.D. fellowship No. 21241753, Chile.

CAI - D4 - P04
Balancing data quantity and quality: Evaluating curation strategies for bioactivity prediction

Carl C.G. Schiebroek[1], Gregory A. Landrum[1], Sereina Riniker[1]
[1]Dept. of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

Building good machine-learning (ML) models to predict the bioactivity of novel chemical matter remains a challenging task. Accurate models require a training set with a large number of diverse compounds and a low level of noise. When extracting data from public databases such as ChEMBL, different levels of curation rigor may be applied, resulting in training sets of varying size, diversity, and, presumably, noise levels. It is not possible to know a priori whether increasing the size of the dataset at the cost of adding more noise improves model generalization. To assess this trade-off, we compare three data curation and modeling approaches: (1) models trained on data for a single target, (2) models trained on target-specific data further restricted to a single set of assay conditions, and (3) multitask learning (MTL) models where each assay condition is treated as a separate task. This MTL approach was designed to bridge the gap between data quantity and quality. Graph neural networks (GNN) and random forests (RF) regressors are evaluated via a leave-assay-out strategy to minimize noise in the test sets. Our results show no meaningful performance differences between these curation strategies, suggesting that for lead-optimization tasks, increasing data quantity at the expense of label consistency does not improve generalization. Notably, the MTL approach also failed to provide a performance advantage. Additionally, we find that GNNs exhibit high seed-dependent variability in connection with the comparatively small training sets common for bioactivity measurements, highlighting the necessity of multi-seed evaluation for robust model assessment.

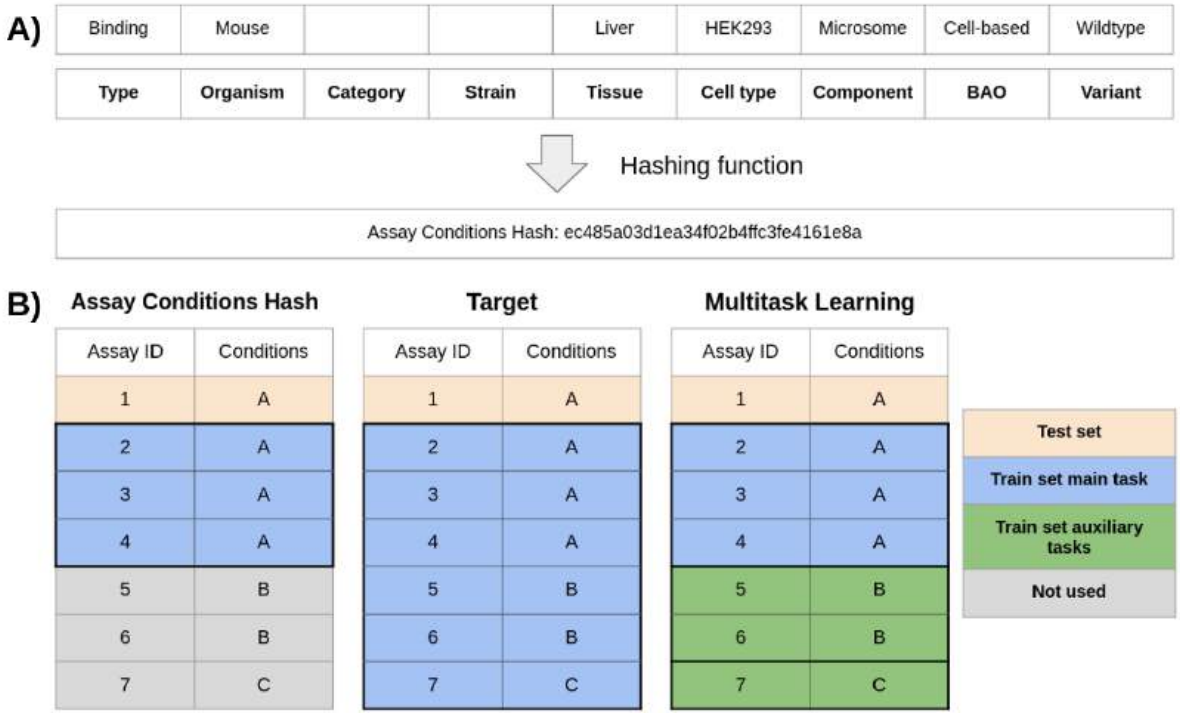

Fig. 1. (**A**): Hashing of assay metadata into the assay conditions hash (ACH). (**B**): Schematic visualization of the curation strategies ACH (left), target (middle), and MTL (right) and the corresponding data splitting. All models are evaluated on the same test set, i.e., in the example assay 1 with conditions A. For ACH, a model is trained on assays 2-4 with the same assay conditions as the test set (conditions A). For target curation, a model is trained on assays 2-7 with mixed assay conditions (conditions A-C). For MTL, a model is trained for three tasks simultaneously (tasks A, B, and C), representing prediction of bioactivity under different assay conditions. Only predictions for the task with conditions corresponding to the test set (condition A) are evaluated on the test set.

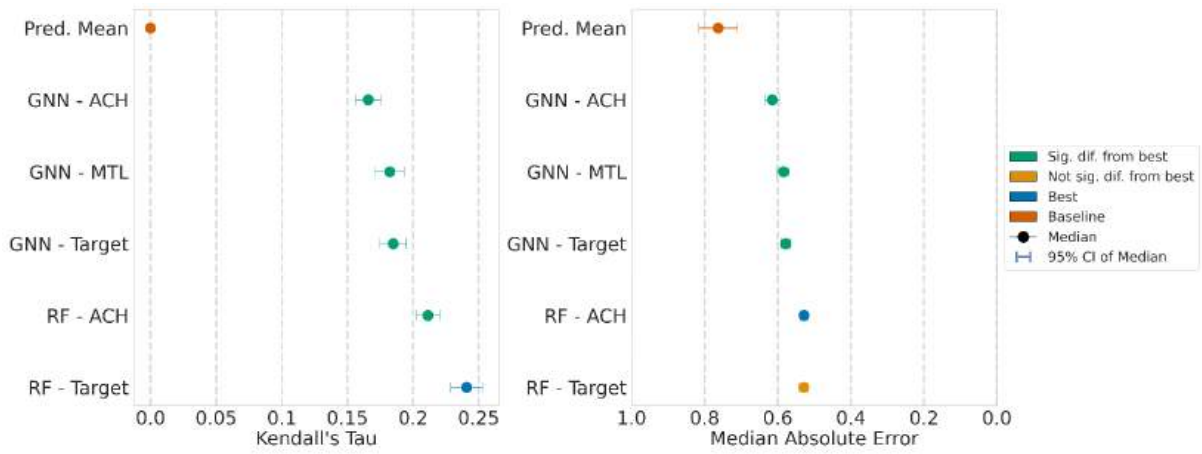

Fig. 2. Comparison of the performance of the ML models over the 422 test sets. The best method is determined based on the best median value of the performance metric. All other methods are compared to this best method using the Conover-Friedman post hoc test with Bonferroni correction for multiple comparisons ($\alpha = 0.05$) as implemented in scikit-posthocs. Performance is put in context of predicting the mean of the (target) training set. Left: Kendall's τ, right: median absolute error (medAE).

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CAI - D4 - P05

Unified data-driven flow regime identification in horizontal and vertical multiphase pipe flows using dynamic pressure signals

Umair Khan[1], Abdullah Shah[1,2], Khaled M. Furati[1,2]
[1]Interdisciplinary Research Center for Refining & Advanced Chemicals, KFUPM, Dhahran, KSA; [2]Dept. of Mathematics, King Fahd University of Petroleum & Minerals, (KFUPM), Dhahran, KSA

Flow regime identification is essential for the reliable operation of gas–liquid multiphase systems widely encountered in chemical and process industries. However, real-time monitoring remains challenging in industrial pipelines where direct visualization is not feasible. In this work, a unified, data-driven framework is developed for flow regime classification in both horizontal and vertical pipe systems using dynamic pressure signals. Dynamic pressure signals are processed using Discrete Wavelet Transform (DWT) to extract multiscale features that capture the underlying flow dynamics. To enable interpretable data representation, multiple dimensionality reduction techniques are evaluated, with Kernel Fisher Discriminant Analysis (KFDA) providing optimal clustering and visualization of flow regimes in a reduced feature space. Machine learning models were then evaluated using an AutoML workflow to identify the best-performing classifier. The proposed methodology is first validated independently for horizontal and vertical flows, achieving testing accuracies of 92.5% and 90.2%, respectively. Building on this, a unified model is developed by integrating both configurations into a single framework. The optimal pipeline (DWT–KFDA–ANN) achieves 100% training accuracy and 92.5% testing accuracy while maintaining strong generalization across flow orientations. The resulting virtual flow regime maps enable direct projection of new pressure data, supporting real-time classification using a moving-window approach. By combining signal processing with interpretable machine learning, this work demonstrates the potential of data-driven methodologies for monitoring and decision support in complex multiphase systems relevant to chemical and energy applications.

Keywords: Two-phase flow; flow regime identification; dynamic pressure; machine learning; AutoML; dimensionality reduction; industrial process monitoring

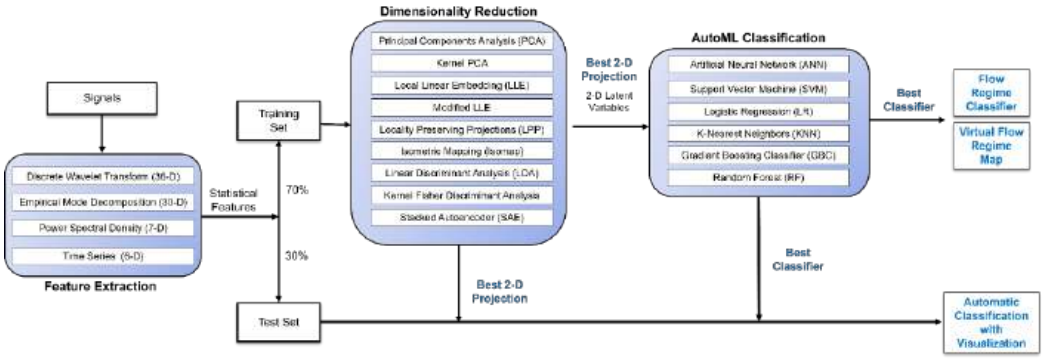

Fig. 1. Overview of the proposed data-driven workflow for flow regime identification. Dynamic pressure signals are processed through feature extraction (DWT), dimensionality reduction (KFDA), and AutoML-based classifier selection to generate a virtual flow regime map for automated classification.

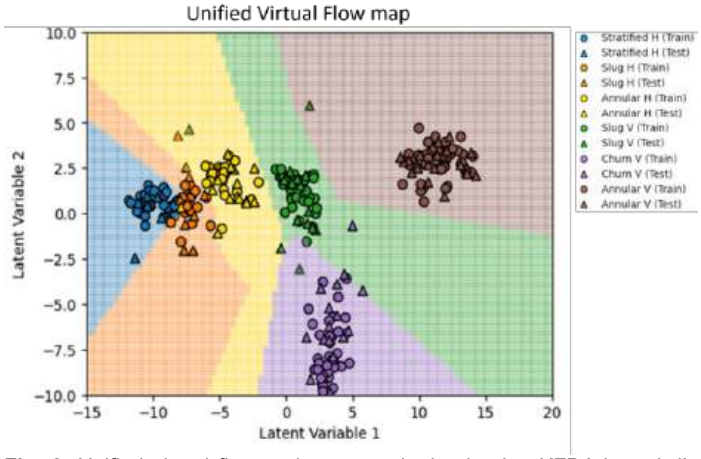

Fig. 2. Unified virtual flow regime map obtained using KFDA-based dimensionality reduction and ANN classification. Data from both horizontal and vertical pipe configurations form distinct clusters with clear decision boundaries, demonstrating the generalization capability of the proposed data-driven framework.

The 10th EuChemS Chemistry Congress

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Posters

Chemistry Meets Biology & Food Science (CBF)

CBF - D1 - P01

Synthesis & structure-activity relationship study on a plant-derived glycoside that attenuates virulence in *Pseudomonas aeruginosa*

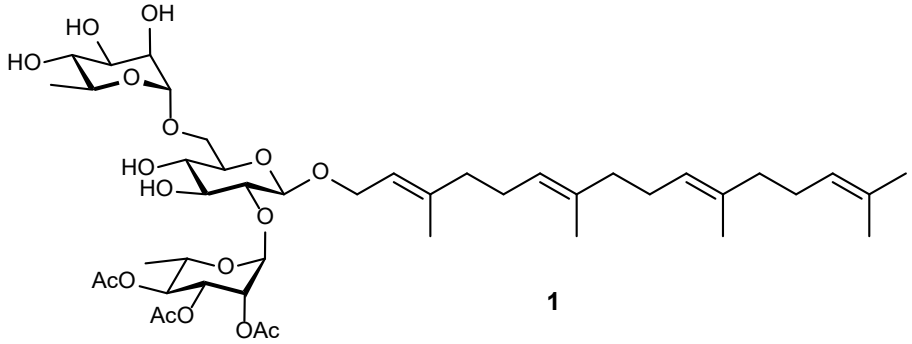
Haris Majstorović[1], Xiaohua Jiang[1], Arnaud Cudré-Mauroux[1], Carmen R. Cori[1], Fabricio Ramírez Cortés[1], Han-Yi Huang[2], Alexandre Persat[2], Rachel Hevey[1]

[1]Molecular Pharmacy, Dept. Pharmaceutical Sciences, University of Basel, Switzerland; [2]Global Health Institute & Institute of Bioengineering, School of Life Sciences, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Pseudomonas aeruginosa is a significant cause of hospital-acquired infections, and in particular poses a severe threat to individuals with cystic fibrosis or compromised immune systems.[1] Its capacity to rapidly develop resistance to antimicrobial drugs has led the World Health Organization to classify it as a pathogen urgently requiring new therapeutic strategies.[2]

During a recent screening campaign of a natural product library, glycoside **1** was observed to attenuate *P. aeruginosa* virulence. To enable a detailed structure–activity relationship study, we developed methodology for the total synthesis of glycoside **1** together with a series of structurally related analogues. This natural product, originally isolated from the plant *Dalbergia oliveri*, is composed of a trisaccharide core linked to a geranylgeraniol-derived diterpenoid aglycone. Synthesis of the compound library presented several challenges, particularly in appending the diterpenoid aglycone and developing an approach for regioselective glycosylation of the different rhamnose residues. Nevertheless, we successfully developed a synthetic route to this complex molecule and its analogues, and with collaborators have been assessing their biological activities to establish well-defined structure-activity relationships.

Acknowledgments: Project supported by the Swiss National Science Foundation (320030-231409) and the University of Basel.



1

Fig. 1. Structure of plant-derived glycoside **1**

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CBF - D1 - P02

Peptide conformation engineering on a chitosan nanowhisker–graphene oxide interface enables high-performance electrochemical detection of food allergen

Jae Hwan Shin[1], Tae Jung Park[2], Chang-Hyung Choi[3], Changyeon Lee[4], Hyunmin Yi[5], Jong Pil Park[1]
[1]Dept. of Food Science and Technology, and GreenTech-Based Food Safety Research Group, BK21 Four, Chung-Ang University, Anseong, Republic of Korea; [2]Dept. of Chemistry, and Research Institute of Chem-Bio Diagnostic Technology (RIChBiDiT), Chung-Ang University, Seoul, Republic of Korea; [3]School of Chemical Engineering, Yeungnam University, Gyeongsan, Republic of Korea; [4]Dept. of Chemical Engineering, Chung-Ang University, Seoul, Republic of Korea; [5]Dept. of Chemical and Biological Engineering, Tufts University, Medford, Massachusetts, USA

Food allergies pose a serious global health risk, as exposure to allergenic proteins can induce rapid and severe immune responses. Therefore, the development of sensitive, selective, and reliable detection strategies for food allergens is critical for ensuring food safety. In this study, we present an affinity peptide-based electrochemical biosensor for the detection of the major food allergen Ara h1, utilizing a chitosan nanowhisker-graphene oxide (CSNW-GO) nanohybrid as a functional sensing interface. The hydrophilic CSNW-GO nanohybrid enhances antifouling properties, surface stability, and electron transfer efficiency, thereby improving overall sensing performance. To elucidate the effect of peptide conformation on target recognition, a phage display-derived cyclic affinity peptide was chemically linearized using tris(2-carboxyethyl)phosphine (TCEP). Comparative structural, electrochemical, and binding kinetic analyses revealed that peptide linearization significantly improved conformational adaptability, charge transfer behavior, and binding affinity toward Ara h1. Based on these results, linear BP1 was selected as the optimal biorecognition element for biosensor fabrication. Oriented immobilization of the peptide was achieved through site-specific EDC/NHS coupling, enabling efficient target capture and signal transduction. The resulting electrochemical biosensor exhibited a broad dynamic detection range, a low detection limit of 0.42 ng/mL, and excellent selectivity against non-target proteins. High reproducibility was demonstrated with a relative standard deviation of 2.3%, confirming the reliability of the sensing platform. Importantly, accurate quantification of Ara h1 was achieved in complex food matrices, highlighting the robustness and practical applicability of the sensor. Overall, this CSNW-GO-assisted, affinity peptide-based electrochemical biosensing platform provides a sensitive and reliable approach for on-site food allergen monitoring and offers a versatile framework for the detection of other protein biomarkers in complex samples.

This research was supported by the National Research Foundation of Korea (NRF) funded by the Korea government (MSIT) (RS-2024-00338698 and RS-2025-02233102).

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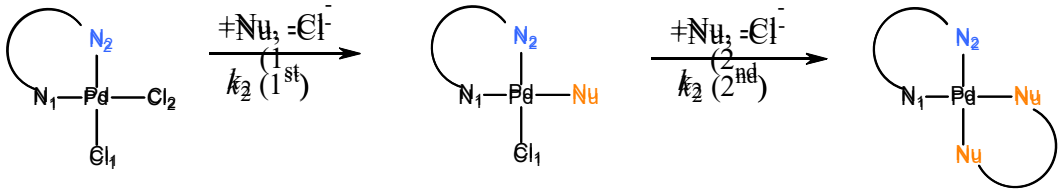
CBF - D1 - P03

Tuning the reactivity of *N,N'*-Pyridyl palladium(II) complexes: A substitution kinetics and DNA/BSA binding study

Pinky Mjwara[1], Siphamandla Sithebe[1], Tshephiso Papo[1]
[1]*University of KwaZulu-Natal, South Africa*

Prompted by the tumor resistance and severe side effects associated with platinum drugs; scientists continue to direct their efforts towards the design of non-platinum metal-based compounds with cytotoxic activity. Amongst several other organometallic compounds being investigated, palladium complexes have emerged as highly functional alternatives, owing to the similarities in characteristics such as softness, size, bond length, and mode of ligand coordination to form complexes, as well as thermodynamic properties. Considering the mechanism of action of platinum(II) complexes when interacting with DNA, proteins and thiol containing biomolecules in target cells, we study the sparsely investigated substitution kinetics, as well as DNA and BSA binding of *N,N'*-pyridyl Pd(II) complexes, viz. dichloro-(N-((pyridin-2-yl)methyl)aniline)palladium(II) (**Pd1**), dichloro-(cyclohexyl-N-((pyridin-2-yl)methyl)-palladium(II) (**Pd2**) and dichloro-(tertbutyl-N-((pyridin-2-yl)methyl)-palladium(II) (**Pd3**). The *N,N'*-bidentate amine ligands and corresponding Pd(II) complexes were synthesized and structurally characterized using ^{1}H-NMR, ^{13}C-NMR, FT-IR spectroscopy and mass spectrometry. The rate of the substitution of the chloride ligands from the complexes by the nucleophiles, i.e., L-Methionine (**L-Met**), L-Cysteine (**L-Cys**) and Glutathione (**GSH**), was studied as a function of nucleophile concentration and temperature using UV–Visible and stopped-flow spectrophotometric techniques, under *pseudo* first-order conditions. The interactions of the palladium complexes (**Pd1-Pd3**) with calf thymus DNA and bovine serum albumin were monitored using UV–Visible spectrophotometry. DFT calculations and in silico binding interactions were performed to elucidate experimental data.



Scheme 1. Mechanism of substitution of chloride ligands by the nucleophile.

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CBF - D1 - P04

Synergistic cancer therapy targeting LAG-3&PD-L1 through co-administration of flavonoid and durvalumab

Konrad Barnowski[1,2], Wen Zhang[3], Judyta Cielecka-Piontek[4], Łukasz Skalniak[1], Jacek Plewka[1]
[1]Faculty of Chemistry, Jagiellonian University, Poland; [2]Doctoral School of Exact and Natural Sciences, Jagiellonian University, Poland; [3]College of Pharmaceutical Science, Zhejiang University of Technology, China; [4]Faculty of Pharmacy, Poznan University of Medical Sciences, Poland

Cancer immunotherapy has changed the landscape of cancer treatment. By using inhibitors of immune checkpoint protein interactions, we reactivate the patient's immune system, enabling it to recognize and destroy cancer cells. The primary target in such therapy is unquestionably the PD-1/PD-L1 interactions, but new emerging proteins are also being considered. For example, blockage of LAG-3 protein interactions with its ligands – MHCII, and FGL1 – proved to also effectively reactivate T cells.

Current state-of-the-art cancer immunotherapy is 2022 FDA-approved synergistic anti-PD-L1 (nivolumab) and anti-LAG-3 (relatlimab) monoclonal antibodies therapeutic, used in the advanced melanoma. Current research is focused on proposing new, small molecule drugs, targeting those proteins. Although such compounds are well-developed in the case of PD-L1 protein, research on LAG-3/ligands interactions inhibitors is in the very beginning phase[1].

In this work, we propose synergistic cancer therapy through co-administration of durvalumab (anti-PD-L1 drug) and a flavonoid. Herein we confirmed direct binding of this molecule to LAG-3 (MST, K_D=4.6 μM) and its blockade of LAG-3/MHCII interactions (HTRF, IC_{50}=19.3 μM), proofing its immunotherapeutic mechanism. We also overcame flavonoid limitations of low aqueous and lipid solubility, by preparing the polymer-based formulation. Such a flavonoid formulation, co-administered with durvalumab, proved to be effective *in vivo* (hPD-L1-MC38 colon cancer tumor model in C57BL/6 mice), reducing tumor weight better than any constituent alone (**Figure**).

Our results provide first *in vivo* proof of synergistic action of anti-PD-L1 monoclonal antibody and small molecules targeting LAG-3/MHCII interactions. These findings open new avenues for developing cost-effective and potentially orally available addition to currently applied cancer immunotherapies.

The research was conducted as part of the OPUS grant “Innovative small molecule inhibitors targeting LAG-3 and the MHCII complex for cancer immunotherapy,” funded by the National Science Centre of Poland (agreement number UMO-2024/53/B/NZ7/02801).

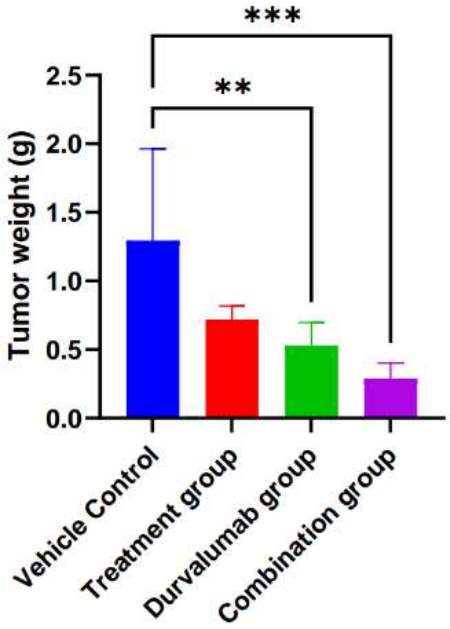

Fig. 1. Synergistic anticancer effect of co-administration of flavonoid and anti-PD-L1 antibody durvalumab on reducing murine tumor weight.

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CBF - D1 - P05
Gold–Selenium carbenes in anticancer therapy

Denys Bondar[1], Steven P. Nolan[1]
[1]UGent, Belgium

The DoNoHarm MSCA Postdoctoral Fellowship introduces a sustainable strategy for the design of gold(I)–N-heterocyclic carbene–selenolate (Au–NHC–Se) complexes as selective and safer anticancer agents.[1] Conventional platinum- and gold-based chemotherapies rely on indiscriminate oxidation and halide activation, which often results in high off-target toxicity.[2] In contrast, DoNoHarm explores solvent-free and green synthetic routes compliant with the MSCA Green Charter, yielding air-stable Au–NHC–Se complexes.
Two complementary synthetic pathways—the weak-base route and elemental selenium insertion—enable fine control over carbene electronics and ligand environments, allowing precise tuning of Au–Se bond lability, a key determinant of biological activity.[3] ^{77}Se NMR chemical shifts correlate with Tolman electronic parameters (TEP), revealing the relationship between donor strength and metal–ligand dynamics.

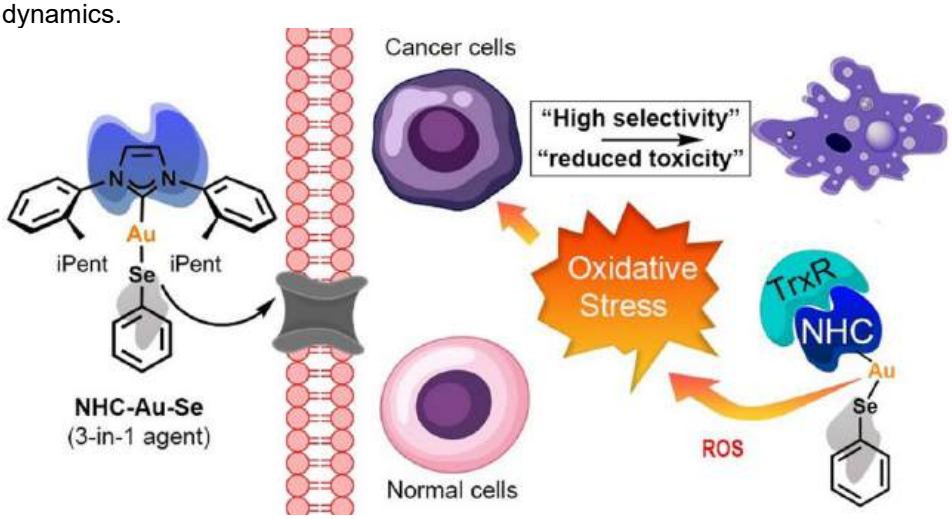

Fig. 2. Concept of the DoNoHarm project.

The lead compound, Au(MonoIPent)SePh (1m), displays sub-micromolar cytotoxicity (IC_{50} ≈ 0.3 μM) and a selectivity index exceeding 13, outperforming both cisplatin and auranofin. Cell-based and cell-free assays confirm thioredoxin reductase inhibition without reactive oxygen species (ROS) overproduction, supporting a controlled soft-metal transfer mechanism rather than oxidative stress—a "potent-without-harm" mode of action. Notably, compound 1m remains active in patient-derived three-dimensional colon and ovarian tumor organoids resistant to oxaliplatin and carboplatin.
By integrating green synthesis, in silico prediction, and in vitro validation, DoNoHarm establishes a circular design paradigm for medicinal organometallics, extendable to Cu- and Ag-NHC analogues, demonstrating that "do no harm" can function as a chemical design principle.

This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie Actions (Grant Agreement No. 101210683 – DoNoHarm).

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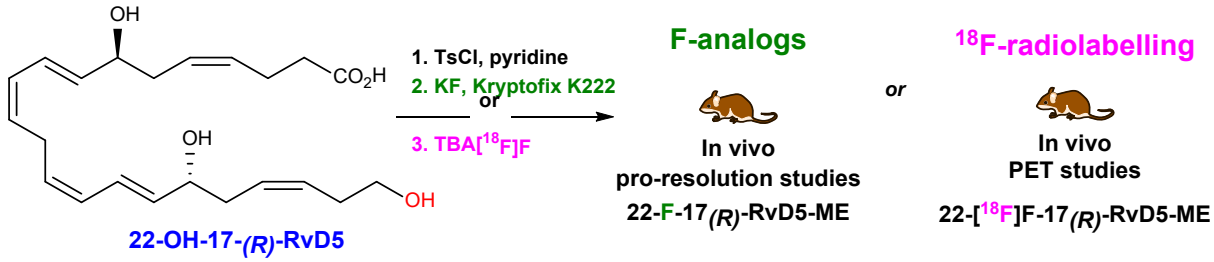
CBF - D1 - P06

Stereoselective synthesis of ^{18}F-labelled specialized pro-resolving mediators

Åshild M. Sørskår[1,2], Amalie F. Reinertsen[1,2], Syed Nuruddin[2,3], Charles N. Serhan[4], Trond V. Hansen[1,2]

[1]Dept. of Pharmacy, University of Oslo, Norway; [2]Norwegian Nuclear Research Centre, Norway; [3]Norsk medisinsk syklotronsenter AS, Norway; [4]Center for Experimental Therapeutics and Reperfusion Injury, Dept. of Anesthesiology, Perioperative and Pain Medicine, Brigham and Women's Hospital, Harvard Medical School, USA

Resolvin D5 (RvD5) is a specialized pro-resolving mediator (SPM) that is biosynthesized from docosahexaenoic acid (DHA) in the body. It has been found that RvD5 reduces inflammatory pain in male mice, but not in female mice.[1] To investigate the mechanisms behind this sex dimorphism, a series of RvD5 analogs will be synthetized, including the ^{18}F-labeled analog that is shown in the scheme below. The radiolabeled compound may be used for positron emission tomography (PET) studies[2], which could provide new insights into how the analogs are distributed *in vivo*, as well as their pharmacokinetics, and target tissue engagement.



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CBF-D1 - P07

Optimization of SPME–GC-MS for volatile profiling and botanical origin discrimination of Portuguese monofloral honey

Maria Beatriz Marmelo[1], Tayse F.F. da Silveira[1,*], Soraia Falcão[1], Lillian Barros[1], Joana S. Amaral[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal

Honey is a natural product with a complex chemical composition, in which aroma and flavor are largely defined by its volatile organic compounds (VOCs). Beyond their contribution to sensory attributes, VOCs constitute valuable chemical markers for honey authenticity, supporting botanical origin discrimination. In this context, solid-phase microextraction (SPME) combined with gas chromatography–mass spectrometry (GC-MS) is a well-established and highly suitable analytical approach for VOC profiling, enabling sensitive and reproducible analysis while minimizing sample manipulation through solvent-free extraction.

In this work, SPME conditions for honey's VOC analysis were optimized, including fiber selection and key extraction parameters. A quality control (QC) sample was prepared by pooling different honeys (orange blossom, rosemary, chestnut, heather, lemon, eucalyptus, arbutus, acacia, thyme, and multifloral) and used throughout the optimization process. Chromatographic separation and extraction parameters—salt addition, sample-to-NaCl solution ratio, homogenization speed, and fiber desorption time—were optimized prior to fiber comparison. Two SPME fibers (DVB/PDMS, 65 µm, and DVB/CWR/PDMS, 50/30 µm) were evaluated under identical incubation conditions (50 °C, 30 min). No significant differences between fibers (p=0.6) in terms of total chromatographic area and number of detected peaks were obtained. Therefore, the DVB/CWR/PDMS fiber was selected based on its broader reported extraction efficiency and its ability to retain a wider range of chemical classes.

A central composite rotatable design (CCRD) was applied to further optimize extraction conditions by systematically evaluating incubation temperature (30–70 °C) and extraction time (5–40 min). The results indicated that higher extraction efficiencies were achieved at longer extraction time (40 min) and higher temperatures (63.9 °C and 70 °C), as evidenced by an increased number of peaks and greater total chromatographic area.

The optimized methodology was applied to the analysis of 30 Portuguese monofloral honey samples, revealing distinct VOC profiles according to the honey's botanical origin.

Acknowledgments: This work was financed by the project "Mel I.D. - Autenticação da origem botânica do mel: metodologias inovadoras baseadas na análise de DNA do pólen e de compostos voláteis com vista à caracterização e valorização de méis portugueses" financed by PNASA 2023-2027, and supported by national funds through FCT/MCTES (PIDDAC): CIMO, UIDB/00690/2020 (DOI: 10.54499/UIDB/00690/2020) and UIDP/00690/2020 (DOI: 10.54499/UIDP/00690/2020); and SusTEC, LA/P/0007/2020 (DOI: 10.54499/LA/P/0007/2020). T.F.F. da Silveira. acknowledges Agenda VIIAFOOD project – Platform for Valorisation, Industrialisation, and Commercial Innovation for Agrifood (C644929456-00000040).

CBF - D1 - P08

Microplastics and nanoplastics in human lung cells: Size-, Polymer-, and exposure model–dependent cytotoxicity

Ricardo Custódio[1], Gabriel Marcondes Ferraz[1], Natasha Caroline Costa Sousa[1], Tamara Teixeira[1], Fillipe Vieira Rocha[1], Roberta Cerasi Urban[1]
[1]Dept. of Chemistry, Federal University of São Carlos, SP, Brazil. roberta.urban@ufscar.br

The widespread production and use of plastics have transformed modern society. While the presence of microplastics and nanoplastics (MNPs) in aquatic environments is well documented, far less is known about atmospheric MNPs and the potential health effects associated with inhalation exposure.[1] This study aimed to provide a preliminary assessment of the cytotoxicity of plastics derived from everyday materials and commercial standards. Human lung fibroblasts (MRC-5) and alveolar epithelial cells (A549) were exposed to different polymers, and cytotoxicity was assessed using the MTT assay.
For direct exposure, 1.5×10^4 cells were added to each well, followed by either a plastic suspension (water or water with 0.01% Tween 20), and for air-liquid-interface exposure, 5.0×10^4 cells were added to each insert, followed by PS suspensions (water). Distinct cytotoxicity patterns were observed depending on polymer type, dose, and particle size (Figure 1).

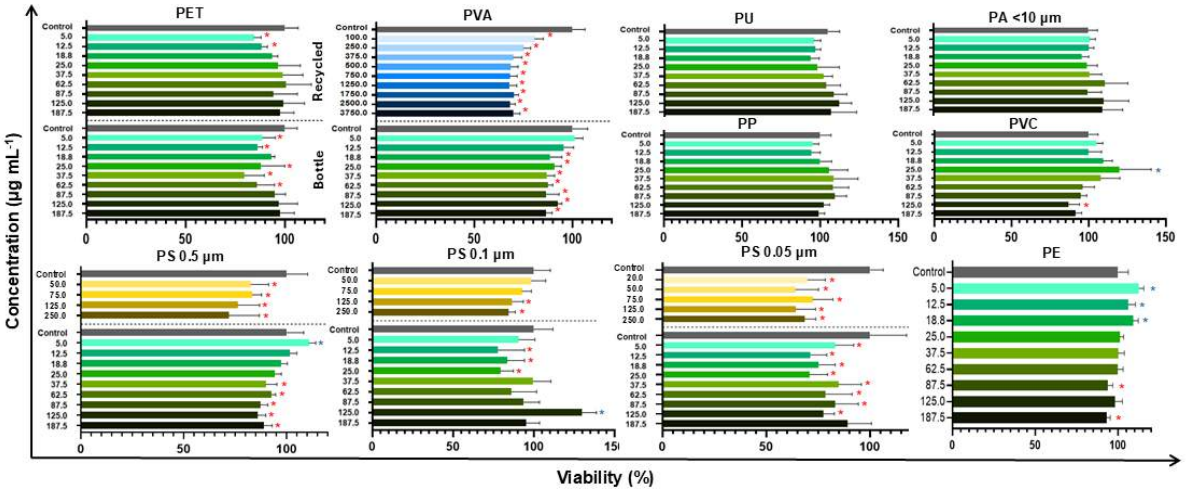

Fig. 1. Cell viability graphs for analyzed plastic particles. Concentrations with statistically lower viability than the control ($p < 0.05$) are marked (*), and those with statistically higher viability ($p < 0.05$) are marked (*)

PET derived from bottles was more cytotoxic than pellet-based PET, possibly reflecting surface differences or the presence of additives acquired during use. PVA showed pronounced, concentration-dependent cytotoxicity, likely related to its higher hydrophilicity and solubility, which may enhance cellular interactions. PU, PP, and PA showed no significant effects, while PVC and PE induced cytotoxicity only at the highest concentrations, possibly due to low surface reactivity and solubility, a greater tendency to agglomerate or lack of surface charge, limiting contact with cells. PS exhibited clear size-dependent toxicity, with 0.05 µm particles causing the greatest effects, highlighting the potential risk posed by ultrafine particles that can interact more extensively with the cell surface. Although no statistically significant differences were observed between exposure models, direct exposure tended to result in higher cytotoxicity, underscoring the need for further studies.

Acknowledgements: CAPES (Financial Code 001), CNPq (148211/2024-0), FAPESP (2022/03087-9, 2022/02876-0, 2023/14823-0, 2023/06768-0) and FINEP (01.22.0182).

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CBF - D1 - P09

Development and validation of analytical performance of ICP-MS blood lead testing method using the ICHM10 new protocol for bioanalytical method

Nardjess Laoufi[1,2], Farida Bouchenak[1,2], Khaled Sobhi[1,2]
[1]Army Central Hospital, Algeria; [2]Faculty of Pharmacy of Algiers, Algeria

Introduction: Lead poisoning, resulting from the ingestion or inhalation of lead and its compounds, is responsible for over 900,000 deaths and 30% of the global burden of idiopathic intellectual developmental disability, The World Health Organization (WHO) has established intervention thresholds of 5 and 45µg/dL for children and adolescents/adults, respectively.
Objectives: This study aimed to validate a method for the determination of blood lead using ICP-MS and a protocol inspired by the ICH M10 guideline specific to bioanalysis.
Materials and methods: A method for quantifying lead in the presence of rhodium as an internal standard (IS) was developed using NexION® 35OX ICP-MS. Argon was used as the plasma gas at a flow rate of 02 L/min. Sample treatment was performed using nitric acid digestion at 90°C for 3 h.
The calibration range from LLOQ (01µg/L) to ULOQ (1500µg/L) included blank and zero samples. Calibration and quality control (QC) solutions at three levels, low at 1.5µg/L, medium at 75.0ug/L, and high at 900.0µg/L, were prepared by overloading whole blood from a standard solution of 1,000±0.002g/L.
The performance parameters validated were the matrix effect, selectivity, response function, fidelity, and accuracy and concentration stability in the matrix, stock, and working solutions tested at +4°C for one month.
Results: The matrix effect test showed signals below 20% (± 5.4%) at the LLOQ and below 5% for IS (± 2.2%). The LQC, MQC and HQC prepared on the six matrices generated a bias in the signal of no more than ±15% (5.3% , 4.2 % and 3.4%) of the nominal value, and a coefficient of variation of less than 15% (7.3%, 6.8% and 7.9%). The calibration range followed a linear regression of the Y=ax+b type, and the calculated concentrations did not deviate by more than 15% from the nominal values (5.5–9.1%).

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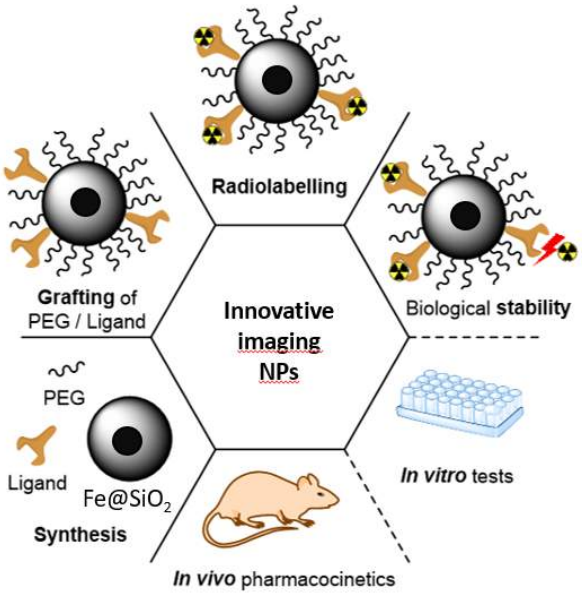
CBF - D1 - P10
Innovative radiolabelled magnetic nanoparticles for dual MRI/SPECT imaging

Maelle Deleuziere[1,2,3], Catherine Amiens[2], Isabelle Quelven-Bertin[3], Franck Desmoulin[3], Clément Morgat[4], Eric Benoist[1]
[1]Synthèse et physico-chimie de molécules d'intérêt biologique, Université de Toulouse, Toulouse, France; [2]Laboratoire de chimie de coordination - CNRS, Toulouse, France; [3]ToNIC, INSERM, Toulouse, France ; [4]Laboratoire INCIA, Bordeaux, France

Combining high resolution MRI and high sensitivity SPECT imaging would allow a more accurate identification and location of small tumors. Dual contrast agents are needed in this context to afford simultaneous acquisition of the images. Silica coated Fe nanoparticles, chosen for their excellent relaxivities in MRI1 have been modified to allow radiolabelling with technetium-99m for SPECT imaging. After carefull characterization and evaluation in vitro, their potential as contrast agents has been assayed on murine cancer models. These modified nanoparticles show potential as diagnostic imaging agents and also as therapeutic agents (in radiotherapy or hyperthermia), offering promising prospects for personalized medicine.



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CBF - D1 - P11

High-throughput serum metabolomics for PFAS toxicity- method development and cohort validation in Belgian residents near a PFAS production plant

Haesong Sher[1], María del Mar Delgado-Povedano[1], Leen Jacobs[1], Ruonan Li[1,2], Ann Colles[3], Eva Govarts[3], Elly Den Hond[4,5], Celine Gys[1] and Adrian Covaci[1]

[1]Toxicological Centre, Dept. of Pharmaceutical Sciences, University of Antwerp, Belgium; [2]Toxicology Dept., School of Public Health, Anhui Medical University, China; [3]VITO Health, Flemish Institute for Technological Research (VITO), Belgium; [4]Provincial Institute for Hygiene (PIH), Belgium; [5]Family Medicine and Population Health, University of Antwerp, Belgium

Exposure to per- and polyfluoroalkyl substances (PFAS) is a major public health concern because of their persistence, bioaccumulation, and toxicity, and has been linked to adverse outcomes, including endocrine disruption, cancer, and metabolic disorders. This study investigates PFAS-associated metabolic alterations in serum from Belgian residents living near a PFAS production plant using untargeted metabolomics. Due to contamination from the plant, these residents experience substantially higher PFAS exposure than the general population. To characterize PFAS exposure-associated metabolic alterations, we applied four complementary metabolomics platforms integrating liquid chromatography–high-resolution mass spectrometry.

Preliminary metabolic profiling of serum was performed to compare adults (20–59 years) divided into two exposure groups within the participants, defined by the 10th percentile (low-exposed) and 90th percentile (high-exposure) of total PFAS concentration (n = 41 per group). Combined univariate and multivariate statistics revealed 38 metabolites. The high-exposed group exhibited downregulation of sphingomyelins and upregulation of phosphatidylglycerols, phosphatidylinositols, and phosphatidylethanolamines, corresponding to moderate perturbations in glycerophospholipid and sphingolipid metabolism. Among the altered metabolites, eight compounds showed moderate correlations ($|r|= 0.2–0.6$) with total PFAS concentration, and six lipids and one amino acid showed individual discriminatory potential between both exposure groups (AUC > 0.6). From these, a panel of five metabolites was selected with around 75% accuracy.

For large-scale cohort application, we developed a high-throughput 96-well serum preparation workflow, comparing different monophasic and biphasic extraction methods. Among them, the selected method is optimized and validated using NIST plasma with rigorous QA/QC (pooled QCs, system suitability testing, blank filtering, and batch correction). We expect to validate preliminary findings in adult (20–59 years) and adolescent (12–17 years) cohorts (20 men and 20 women per exposure group for each cohort) residing within 5 km of the PFAS production plant, stratified by total PFAS concentrations and sex, using univariate/multivariate analyses.

CBF - D1 - P12
Green extraction of pomegranate peel unlocks ellagitannin-driven longevity pathways

Emily Schifano[1], Daniela Uccelletti[1], Stefania Cesa[2*], Francesco Cairone[2]
[1]Dept. of Biology and Biotechnologies Charles Darwin; [2]Dept. of Chemistry and Technologies of Drug, "La Sapienza" University of Rome, Rome, Italy

The valorization of agri-food waste through sustainable extraction represents a key challenge for circular bioeconomy and green chemistry. Pomegranate peel (*Punica granatum* L.), an abundant processing by-product, was investigated as a renewable source of ellagitannins using environmentally benign solvent systems (water, ethanol, and EtOH/H_2O mixtures). Solvent tuning markedly influenced extraction efficiency, with a 70:30 hydroalcoholic mixture yielding the highest recovery (~28%) and selectively enriching punicalagin, identified as the dominant constituent by HPLC-DAD analysis. These findings align with previous evidence highlighting intermediate-polarity solvents as optimal for phenolic extraction from plant matrices [1,2].
Hydroalcoholic extracts exhibited superior antioxidant capacity (DPPH, FRAP), confirming the strong relationship between solvent-driven composition and redox activity. The extract with the richest phytochemical profile was evaluated *in vivo* using *Caenorhabditis elegans* model, a conserved model for studying stress-response modulation by dietary polyphenols [3].
Supplementation extended lifespan and improved key health-span indicators, including locomotion, feeding behavior, muscle organization, and intestinal integrity. Molecular and reporter analyses demonstrated activation of the SKN-1/NRF2 detoxification pathway, with increased expression of *gst-4*, *sod-3*, and *skn-1*, and loss of benefit in *skn-1* mutants, indicating a mechanism based on adaptive stress signaling rather than direct radical scavenging. The extract further reduced age-associated mitochondrial ROS and transiently enhanced respiratory activity, consistent with hormetic responses widely associated with polyphenol-mediated longevity.
By integrating green extraction design, analytical profiling, and functional validation, this study demonstrates that mild, scalable hydroalcoholic processing can convert food waste into a source of bioactives capable of modulating conserved redox pathways. The approach provides a chemically sustainable strategy for transforming agricultural residues into high-value ingredients for nutraceutical and functional applications.

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CBF - D1 - P13

Pesticide residues in commercial honey samples: Application of a validated analytical method and chemometric interpretation

Robert Cholewa, Dawid Strzelecki, Paulina Łukaszewicz, Łukasz P. Haliński
University of Gdansk, Poland

Neonicotinoids and fungicides are widely used in modern agriculture and are frequently applied simultaneously to the same crops. Although fungicides alone are generally considered to be of low toxicity to insects, they can significantly increase the acute and chronic toxicity of neonicotinoids to bees, for example by affecting detoxification mechanisms. Consequently, their simultaneous determination is essential for a reliable assessment of the actual exposure of bees to pesticide residues present in agricultural environments. Honey, produced from nectar and pollen collected by bees over extensive foraging areas, represents a suitable and integrative matrix for monitoring the presence of pesticides used in the agriculture.

In this study, modern matrix-induced sugaring-out liquid–liquid extraction (SULLE) methods with the addition of an organic modifier were developed and optimized for the isolation of pesticides from honey samples. The procedures enabled effective separation of target analytes from matrix interferences, resulting in improved recoveries, repeatability, and overall analytical performance. Optimization of the extraction conditions involved the use of central composite designs (CCD) with the organic phase volume, modifier concentration, and sample cooling time as factors examined to ensure efficient extraction. Finally, analytes were determined using LC–MS/MS.

The validated method was applied to the analysis of 108 commercial honey samples originating from different regions worldwide, with a substantial proportion of samples produced within the EU. Pesticide residues were detected in the majority of the samples analyzed. The resulting dataset was further evaluated using chemometric tools, including principal component analysis (PCA), to investigate similarities between samples and to identify general contamination patterns. The proposed analytical approach constitutes a practical tool for large-scale monitoring studies as well as for quality control of honey and other bee products. Compared to the standard QuEChERS approach, the developed method offers shorter sample preparation time, high sensitivity, and a more favorable cost balance.

CBF - D2 - P01
Molecular characterization of *Dendronephthya gigantea* phenylalanine ammonia-lyase

Yu-Ting Yu[1], Lu-Sheng Hsieh[1]
[1]Department of Food Science, Tunghai University, Taiwan

Phenylalanine ammonia-lyase (PAL; EC 4.3.1.24) catalyzes the non-oxidative deamination of L-phenylalanine to produce *trans*-cinnamic acid (*t*-CA) and ammonia. PAL is a key protein in enzyme replacement therapy for phenylketonuria (PKU), the conversion of excess phenylalanine into the non-toxic *t*-CA effectively reduces metabolic burden in patients. In addition, *t*-CA possesses considerable industrial and pharmaceutical potential and is in high market demand. However, its natural yield is limited, extraction from natural sources causes environmental damage, and chemical synthesis imposes substantial environmental burdens. Therefore, the development of an environmentally friendly and cost-effective biosynthetic production platform is highly desirable. PAL is known to be widely distributed in higher plants and present in a limited number of fungi and prokaryotes, but is absent in animals. In this study, a putative *DgPAL* gene was identified from the soft coral *Dendronephthya gigantea* through database mining. We used metabolic engineering strategies to heterologously express the DgPAL in *Escherichia coli* BL21 strain, establishing a microbial platform for the production of DgPAL protein as well as *t*-CA derivatives. Our results showed that DgPAL protein can be successfully overexpressed in *E. coli* and purified as an active enzyme. The recombinant DgPAL protein exhibited maximal catalytic activity at 50 °C and pH 7.5. These findings confirm the functional expression and applicability of DgPAL protein produced in *E. coli*, highlighting its potential for large-scale PAL production and for the sustainable biosynthesis of *t*-CA through metabolic engineering.

This study was supported by a reserach from the National Science and Technology Council, Taiwan (NSTC 113-2313-B-029-002-MY3 for LSH).

CBF - D2 - P02
Crystallization-assisted and mechanoenzymatic synthesis of chiral amines using transaminases

Julie Dullier[1], Damien Debecker [2], Tom Leyssens[3], Johan Wouters[1]
[1]Chimie Biologique Structurale (CBS), University of Namur, Belgium; [2]Faculty of bioengineers (ARGO), University of Louvain, Belgium; [3]Faculty of sciences, Dept. of chemistry, University of Louvain, Belgium

Chiral amines are essential building blocks in many fields such as pharmaceuticals and agrochemicals.[1] The aim of this project is to develop a sustainable and innovative approach for the synthesize of chiral amines via transamination using transaminases (TAs). These enzymes catalyze the reversible conversion of ketones or aldehydes into amines using an amine substrate, also called an amine donor, in the presence of the cofactor pyridoxal-5'-phosphate (PLP).[1] When prochiral ketones are used, individual enantiomers can be selectively obtained by employing either (S)- or (R)-selective transaminases (Figure 1). Despite their advantages in terms of sustainability and selectivity, transaminase-catalyzed reactions are often limited by thermodynamically unfavorable equilibria.[2]
The main objective of this work is to improve and design an original biocatalytic synthesis of sertraline, the active ingredient of Zoloft®, widely prescribed for the treatment of depression and anxiety disorders.[3] The proposed synthetic pathway is based on the asymmetric amination of a desmethylsertraline precursor, namely (S)-4-(3,4-dichlorophenyl)-3,4-dihydronaphthalen-1(2H)-one. A synthetic scheme is proposed in Figure 2.
The first part of this project will focus on identifying optimal conditions for the synthesis of desmetylsertraline from its precursor. This will involve screening different TAs and evaluating various amine donors to identify the most effective catalytic system. Subsequently, the biocatalytic process will be optimized by coupling it with in situ crystallization, thereby shifting the reaction equilibrium toward product formation through precipitation.[4]
The second part of this work will explore the feasibility of performing this transformation under mechanoenzymatic conditions. This approach aims to further enhance the sustainability of the process by reducing solvent use and enabling alternative reaction environments for enzymatic catalysis.[5]

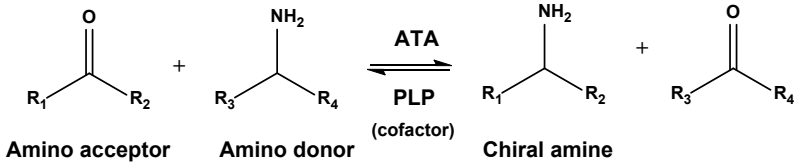

Fig. 1. Asymmetric synthesis of chiral amine with amine transaminase (TA)

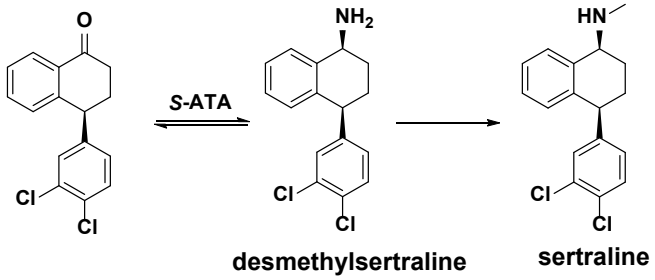

Fig. 2. Biocatalytic transamination-based synthesis of desmethylsertraline from (S)-4-(3,4-dichlorophenyl)-3,4-dihydronaphthalen-1(2H)-one, followed by conversion to sertraline

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CBF - D2 - P03

New water-soluble La(III) and Ce(III) complexes as structurally defined candidates for anticancer applications

Aurel Tăbăcaru[1], Andreea Veronica Botezatu[1], Rodica Mihaela Dinică[1], Simona Butan[1], Mariana Bușilă[1], Fernanda Marques[2], Sergiu Shova[3]

[1]„Dunărea de Jos" University of Galați, Romania; [2]Centro de Ciências e Tecnologias Nucleares (C[2]TN) and Dept. de Engenharia e Ciências Nucleares, Instituto Superior Técnico, Universidade de Lisboa, Portugal; [3]„Petru Poni" Institute of Macromolecular Chemistry, Romania

Lanthanide(III) complexes continue to attract significant interest in medicinal inorganic chemistry due to their high coordination flexibility and emerging antitumor potential.[1-4] Herein, the synthesis and structural characterization of two new lanthanide(III) complexes of La and Ce are reported. Reaction of $Ln(NO_3)_3 \cdot 6H_2O$ (Ln = La, Ce) with 2,2′-bipyridyl (bpy) and quercetin in a 1:1:1 molar ratio, in ethanol at 80 °C, afforded two discrete, water-soluble mononuclear complexes with the stoichiometric formula $[La(bpy)(NO_3)_5](Hbpy)_2$ and $[Ce(bpy)_2(NO_3)_3]$. Although quercetin is present in the reaction medium, it does not coordinate to the lanthanide ions. However, its presence appears to influence the self-assembly process leading to the isolated products. Single-crystal X-ray diffraction reveals that the La(III) complex is ionic, consisting of a twelve-coordinated La^{3+} center bound to one neutral chelating bpy ligand and five bidentate nitrate groups, resulting in a distorted icosahedral coordination geometry. Charge balance is provided by two monoprotonated bpy cations located outside the primary coordination sphere. In contrast, the Ce(III) complex is neutral and features a deca-coordinated Ce^{3+} ion coordinated by two chelating bpy ligands and three bidentate nitrate anions, adopting a distorted bicapped square-antiprismatic geometry. These lanthanide complexes could be important as anticancer agents. Therefore, their cytotoxicity in relevant cancer cells, the mechanisms of cell death (apoptosis/necrosis), oxidative stress and inhibition of cellular vital enzymes will be evaluated. The present study highlights the influence of reaction conditions and auxiliary components on lanthanide complex formation, and provides structurally well-defined candidates for further biological investigation.

Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-IV-P2-2.1-TE-2023-1242, within PNCDI IV, contract no. 100TE/03.01.2025.

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CBF - D2 - P04
Development of novel JAK degraders via PROTAC technology

Dongyun Shin[1], Eo-Jin Park[1], Juyeun Lee[2]
[1]Gachon University, South Korea; [2]Seoul National University, South Korea

Myelofibrosis (MF) is a severe myeloproliferative neoplasm characterized by bone marrow fibrosis and anemia, primarily driven by the dysregulation of the JAK/STAT signaling pathway. While JAK2 inhibitors such as Ruxolitinib are the standard of care, they are often limited by dose-dependent toxicities, particularly the exacerbation of anemia due to the suppression of erythropoietin signaling. To overcome the limitations of traditional occupancy-driven inhibitors, this study focuses on the development of JAK2 degraders using Proteolysis-Targeting Chimera (PROTAC) technology.[1]
We designed and synthesized a series of novel PROTACs by conjugating a JAK2-binding moiety, derived from the inhibitor Momelotinib, to ligands for E3 ubiquitin ligases (Cereblon or VHL) via various linkers.[2,3] Momelotinib was selected as the warhead due to its dual inhibition of JAK1/2 and ACVR1, which offers potential benefits for improving anemia. The objective was to induce the selective ubiquitination and subsequent proteasomal degradation of JAK2, thereby abolishing its pathogenic signaling more effectively than simple inhibition.
This presentation will detail the synthesis of these heterobifunctional molecules and the resulting Structure-Activity Relationship (SAR) data. We evaluated the biological activity of the synthesized library, including their anti-proliferative efficacy in cell models. Our findings demonstrate the feasibility of targeted JAK2 degradation and suggest that this modality may offer a superior therapeutic window for MF patients by addressing the shortcomings of existing kinase inhibitors.

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CBF - D2 - P05

Hydrotrope-modulated AGA hydrogels as sustainable nanocarriers for molecules of different hydrophobicity

Eva Mueller[1], Patrick Denk[1], Lea Sammet[1], Didier Touraud[1], David Diaz-Diaz[2], Werner Kunz[1]
[1]University of Regensburg, Institute of Physical Chemistry, Germany; [2]University of La Laguna, Dept. de Química Orgánica, Spain

The sustainable solubilization and encapsulation of hydrophobic molecules remain major challenges in formulation science. Hydrogels based on ammonium glycyrrhizic acid (AGA) are promising biodegradable and biocompatible matrices, yet their intrinsic ability to solubilize poorly water-soluble compounds is limited. Here, short-chain alcohols are investigated as hydrotropes and co-solvents to tailor the supramolecular organization, acid-base equilibria, and nanocarrier performance of AGA/water/alcohol hydrogels. Hydrotrope-dependent pKa shifts and ionization states of AGA, and gel structure and dynamics were determined.

We recently showed that ethanol, characterized by low relative permittivity and pronounced amphiphilicity, induces increased apparent pKa values and enhanced dissociation of glycyrrhizic acid due to fibril intercalation, increased spacing of carboxyl groups, and hydrotropic effects. These opposing contributions promote the formation of long, entangled fibrillar networks at moderate alcohol contents, but lead to fibril fragmentation into micelle-like aggregates at higher concentrations.[1] Isopropanol exhibits an even stronger effect, consistent with its lower permittivity and higher hydrotropic efficiency. In contrast, glycerol causes only modest pKa shifts and primarily stabilizes AGA ions through extensive inter- and intrafibrillar hydrogen bonding, resulting in a moderately developed but progressively strengthened network with increasing glycerol content.

Accordingly, the solubilization and nanocarrier efficiency was probed for solutes of varying hydrophobicity. Complementary studies with the poorly soluble natural sweetener rebaudioside A (RebA) demonstrate up to a 25-fold solubility enhancement and thermoreversible gelation in the presence of AGA, surpassing conventional surfactants. Scattering and recovery experiments support a dual-aggregate scenario involving partial co-assembly within AGA fibrils and RebA-rich spheroidal domains, comparable to ethanol.

Thus, AGA/short-chain alcohol hydrogels are tuneable, sustainable solubilizers and nanocarriers with potential applications in food, cosmetics and drug delivery.

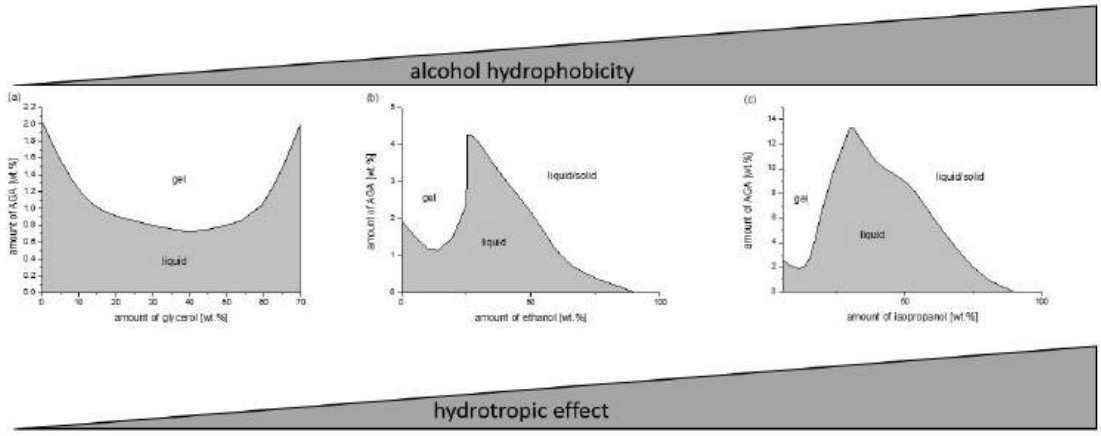

Fig. 1. Impact of different alcohols on the gelation behaviour of AGA.

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CBF - 2 - P06

Combined computational & experimental approach to design & synthesize new molecules having anti-tuberculosis properties

Prashant. B, Singh[1], Ajoy Kapat[1,*]
[1]Dept. of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence, Delhi-NCR, India

Tuberculosis (TB) remains a major global health challenge, affecting approximately **10 million individuals annually** and causing an estimated **1.5 million deaths worldwide**. Nearly **one-third of the global population carries latent Mycobacterium tuberculosis infection**, representing a substantial reservoir for future disease [1]. The increasing prevalence of **multidrug-resistant (MDR-TB)** and **extensively drug-resistant tuberculosis (XDR-TB)**—defined by resistance to first-line agents and, in the case of XDR-TB, additional resistance to key second-line drugs—poses a serious threat to TB control efforts [2]. The recent approval of the **pretomanid–bedaquiline–linezolid (BPaL)** regimen by the **U.S. Food and Drug Administration** for MDR-TB and XDR-TB marks a significant therapeutic advance. However, current treatment options remain constrained by **prolonged regimens, substantial toxicity, drug–drug interactions, and poor patient adherence**, underscoring the urgent need for safer and more effective anti-TB therapies [1]. At present, numerous targets have been identified for the development of improved anti-TB medicines, among which Decaprenylphosphoryl-β-D-Ribose-2'-Epimerase-1 (DprE1), a flavoenzyme, is a major target for anti-TB therapy. The crucial role of DprE1 is the biosynthesis of the mycobacterium cell wall. Recently, the two covalent inhibitors of DprE1, benzothiazinone class of compound (*BTZ-043*) and piperazinobenzothiazinone derivative (*PBTZ-169*) have entered phase 2 clinical trials to treat pulmonary TB [3].

The major challenge lies in the synthesis of benzothiazinone compounds. Over the past decade, the number of BTZ-043 synthesis steps decreased from 7 to 5, while yields increased only marginally from 36% to 42% [4]. In this project, studying the structure-activity relationship [5] of BTZ-043, and analysing the structure responsible for inhibition of DprE1, the synthetic challenge was tackled by developing a highly efficient sequential conjugate addition reaction of substituted thiosalicylic acid and substituted phenyl propargylic ketone [6]. The comparative docking score of model substrate (-8.7kcal/mol) and BTZ-043 (-9.2 kcal/mol) exhibited the comparative binding affinity towards DprE1 enzyme. The model substrate maintained greater conformational stability than the control, as indicated by lower RMSD fluctuations. MM-GBSA calculations further confirmed the docking results, with the model substrate exhibiting the most favourable binding free energy [7].

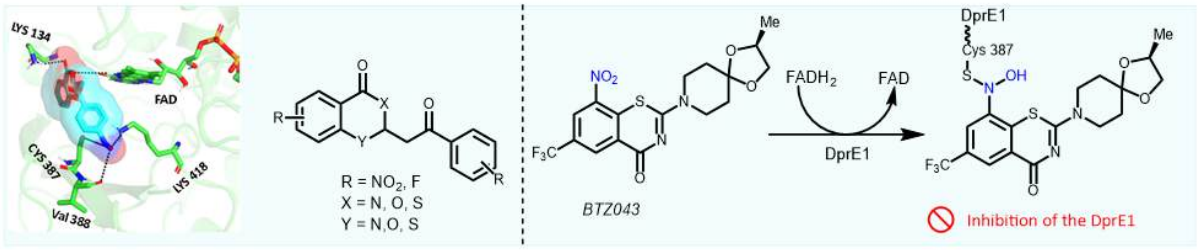

Fig. 1. Comparative analysis of model substrate and BTZ043.

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CBF - D2 - P07

Physicochemical characterization and *in vitro* digestibility of cocoa pod husk extract for application in edible gums

Lili Dahiana Becerra[1], Cristian Blanco-Tirado[1]
[1]Grupo de Investigación en Fisicoquímica Teórica y Experimental, Universidad Industrial de Santander, Colombia

The utilization of cocoa (Theobroma cacao L.) by-products represents a promising strategy for developing functional ingredients in the food industry. Cocoa pod husk is rich in bioactive compounds, including polyphenols and methylxanthines, which exhibit antioxidant properties, making it suitable for incorporation into edible gums. In this study, the physicochemical characterization of cocoa pod husk was performed, evaluating total phenolic content and antioxidant capacity using ABTS and DPPH assays. The extract was prepared under controlled extraction conditions suitable for functional food applications. The results indicated a high content of total phenolics and substantial antioxidant activity. Major bioactive components identified included caffeine, theobromine, catechin, and epicatechin. The cocoa pod husk extract was subsequently subjected to an in vitro gastrointestinal digestion following the standardized INFOGEST protocol[1,2]. Polyphenol release was progressive throughout digestion, with the highest liberation observed during the intestinal phase. Notably, caffeine and theobromine were gradually released, indicating their potential availability for absorption. Considering its application in edible gums, the polymeric matrix may contribute to controlled release by providing partial protection under gastrointestinal conditions. These findings demonstrate that a significant fraction of bioactive compounds remains available after digestion, retaining part of their antioxidant capacity. This work contributes to the valorization of cocoa by-products within a circular economy framework, emphasizing their potential to enhance food functionality and reduce waste in the cocoa industry.

This work was supported by research project 4625, funded by the Vice-Rectory for Research and Extension of Universidad Industrial de Santander (UIS). The authors acknowledge the institutional facilities and technical assistance provided during the experimental development.

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CBF - D3 - P01

Nanoparticle-based lateral flow immunoassays for detecting marine biotoxins in seafood: A systematic review of trends in development over two decades

Perveen Akhtar [1,2*], Hugh J. Byrne [2], Furong Tian[1,2], Bilal Javed [1,2*]
[1] School of Food Science and Environmental Health, TU Dublin Grangegorman, Ireland
[2] Physical to Life Sciences Research Hub, TU Dublin, Ireland

Marine and freshwater biotoxins threaten public health and seafood safety due to their tendency to accumulate in fish and shellfish. This systematic literature review summarises findings from 51 peer-reviewed studies published between 2004 and 2025 that focus on nanoparticle-enhanced lateral flow immunoassays (LFIAs) for toxin detection. Gold nanoparticles (AuNPs) were by far the most used label, employed in ~75% of studies, which consistently delivered the lowest limits of detection (LODs) as low as 0.03 ng/ml for okadaic acid detection. Despite increasing concerns over the co-occurrence of multiple toxins, ~88% of the studies were based on single-analyte detection, only ~12% employing multiplexed approaches. Statistical analyses of the studies, namely Kruskal–Wallis, Dunn's post hoc, correlation, and regression analysis, revealed meaningful trends. LODs have significantly improved over time, a marked reduction being observed after 2016. Kruskal–Wallis and Dunn's post hoc tests showed significant differences across variables such as nanoparticle size, assay duration, and toxin recovery. Spearman correlation results identified a moderately significant negative correlation of LOD with publication year ($\rho = -0.458$, $p < 0.001$), and a weaker significant correlation of LOD with assay time ($\rho = -0.301$, $p = 0.018$), while linear regression analysis identified publication year ($R^2 = 0.2441$, $p < 0.0001$) and nanoparticle size ($R^2 = 0.1072$, $p = 0.0264$) as significant predictors of assay sensitivity. Overall, this review underscores the central role of nanoparticle engineering, simplified assay workflows, and optimized design strategies in improving LFIA performance. The findings provide a valuable roadmap for advancing the development of portable, sensitive, and scalable biosensing platforms for marine toxin monitoring and seafood safety surveillance.

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CBF - D3 - P03

Breaking the NMDAR/TRPM4 protein dialogue: Small-molecule disruptors as a novel neuroprotective strategy for ischemic stroke

Katarzyna Szafrańska[1,2], Maciej Czuba[1], Monika Marcinkowska[1], Barbara Mordyl[1], Monika Głuch-Lutwin[1], Bartosz Pomierny[1]

[1]Jagiellonian University Medical College, Faculty of Pharmacy; Poland; [2]Jagiellonian University Medical College, Doctoral School of Medical and Health Sciences, Poland

Acute ischemic stroke remains one of the leading causes of death and long-term disability worldwide, yet effective neuroprotective therapies are still lacking. For decades, therapeutic strategies focused on global inhibition of *N*-methyl-D-aspartate receptors (NMDARs) to prevent glutamate-driven excitotoxicity.[1] Despite strong preclinical rationale, clinical trials of NMDAR antagonists consistently failed due to severe adverse effects and increased mortality, highlighting the indispensable physiological role of NMDAR signaling in neuronal survival and recovery.[2] Recent discoveries demonstrated that excitotoxic neuronal death is mediated specifically by an extrasynaptic NMDAR/TRPM4 signaling complex. Selective disruption of this protein–protein interaction suppresses pathological signaling while preserving the essential synaptic functions of NMDARs (Figure 1.), establishing the NMDAR/TRPM4 complex as a promising target for next-generation neuroprotective therapies.[3]

However, the chemical space of known disruptors remains extremely limited and is dominated by a narrow class of *N¹*-benzyl-*N¹*-ethylethane-1,2-diamine derivatives with insufficient pharmacokinetic and ADMET characterization.[3] To address this challenge, our project focuses on the medicinal chemistry-driven development of novel small-molecule disruptors of the NMDAR/TRPM4 complex.

Several new compounds have been designed, synthesized, and evaluated *in vitro*. Initial biological studies demonstrated promising activity for selected derivatives, supporting further optimization and structure–activity relationship investigations. By combining synthetic organic chemistry with pharmacological screening, this work aims to expand the repertoire of selective NMDAR/TRPM4 disruptors and advance the development of safer and more clinically viable neuroprotective agents for acute ischemic stroke.

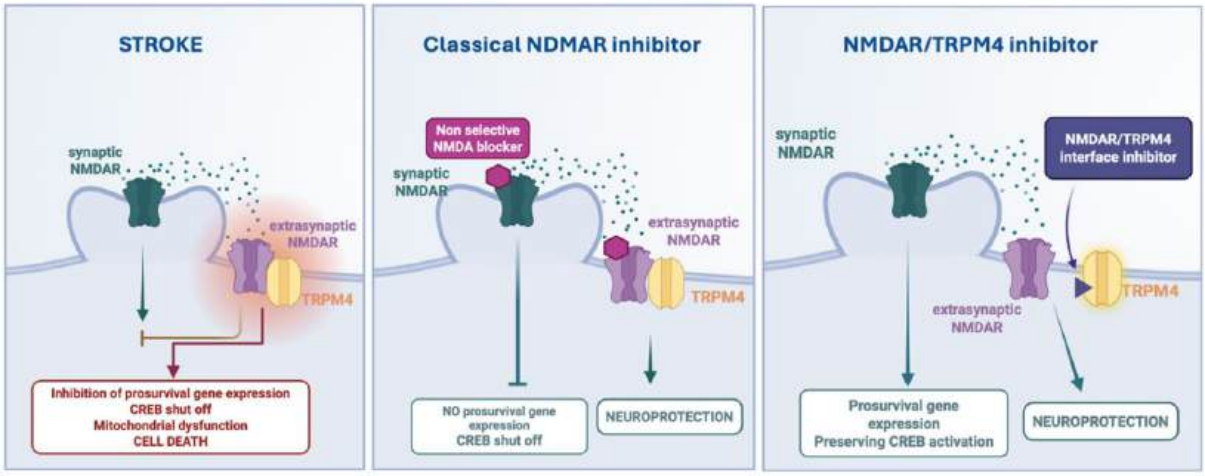

Fig. 1. Classical NMDAR neuroprotection versus selective blockade of NMDAR/TRPM4 interface.

Research funded by National Science Centre, Poland. Projects number 2023/50/E/NZ7/00586 and 2025/57/N/NZ7/02201.

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CBF - D3 - P04
Method validation for the determination of pyridate in agricultural commodities

Yun Mi Chung[1], Ayeong Ma[1], Jang Duk Choi[1]
[1]Hazardous Substances Analysis Division, Gwangju Regional Office of Ministry of Food and Drug Safety, Gwangju, Korea

Pyridate is a photosynthesis-inhibiting herbicide that suppressed weed growth by blocking electron transport in Phtosystem II. Accoding to CODEX, EC(Europe), EPA(USA), JFCRF(Japan) and PMRA(Canada), maximum residue limits(MRLs) of pyridate are regulated based pyridate, pyridafol(hydrolysis products of pyridate), and pyridafol-O-glucoside(glycosides of pyridafol), expressed as pyridate equivalents, with MRLs ranging from 0.03-10 mg/kg for various agricultural commodities. In Korea, analytical method for pyridate is required as the residue definition is expected to include the parent compound and its metabolites.
In this study, an analytical method verified by the National Institute of Food and Drug Safety Evaluation(NIFDS) was independently validated for the safety management of pyridate and its metabolites. Five representative agricultural commodities(brown rice, potato, soybean, citrus and green pepper) were selected for this method validation. Samples were treated with 1N NaOH and extracted with acetonitrile, followed by acid hydrolysis with 1N HCl at 70℃ and dehydration using $MgSO_4$ and NaCl. The extract was purified using disperse solid phase extraction(d-SPE) kit with anhydrous $MgSO_4$ and C_{18}, and then analyzed by LC/MS/MS. The matrix-matched calibration curves showed good linearity, with coefficients of determination(R^2) greater than 0.99. The limit of detection and the limit of quantification was confirmed to be below 0.003 mg/kg and 0.01 mg/kg, respectively. The method demonstrated acceptable recoveries and precision at three spiked levels(LOQ, 10×LOQ, 50×LOQ, n=3), with recovery values of 89.8-103.6% for pyridate, 80.8-108.8% for pyridafol, and 75.8-96.0% for pyridafol-O-glucoside, and the relative standard deviation was less than 4.7% or less.
These results confirm that the method complies with the residue analysis criteria set forth by the Codex guidelines(Codex Alimentarius Commission, CAC/GL 40). Based on these results, the proposed analytical method has been demonstrated to be suitable for the detection and quantification of pyridate. It can be utilized as a reference method for establishing MRLs.

CBF - D3 - P05

Impact of cation alkyl chain length on the antimicrobial efficacy of 1-alkyl-3-methylimidazolium ionic liquids

Utibe B. Akpan[1*], Ogechukwu V. Ezeh[2], Wei Han[1], King Lun Yeung[1,2]

[1]Division of Environment and Sustainability: [2]Dept. of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Hong Kong SAR, China

The antimicrobial application of ionic liquids (ILs) have become a significant research focus due to their excellent features such as low volatility, high thermal stability, and tunable properties.[1] This study investigates the antimicrobial efficacy of 1-alkyl-3-methylimidazolium chloride ($C_nMIM[Cl^-]$) and 1-alkyl-3-methylimidazolium tetrafluoroborate ($C_nMIM[BF_4^-]$) ionic liquids at varying alkyl chain lengths against *Staphylococcus aureus* and *Pseudomonas aeruginosa* in both liquid-phase and dry-phase tests on High Efficiency Particulate Air (HEPA) filters. Bactericidal activity increased with the length of the alkyl chain and was concentration dependent. Additionally, bactericidal activity was higher in liquid-phase (figure 1) compared to dry phase with IL coated HEPA filters (figure 2), a disparity which may be attributed to the enhanced solubility and mobility of the ionic liquids in the liquid phase, which allows for more effective interaction with bacterial cells. This could have implications for developing ionic liquid disinfectant formulations for different applications where antimicrobial properties are needed.

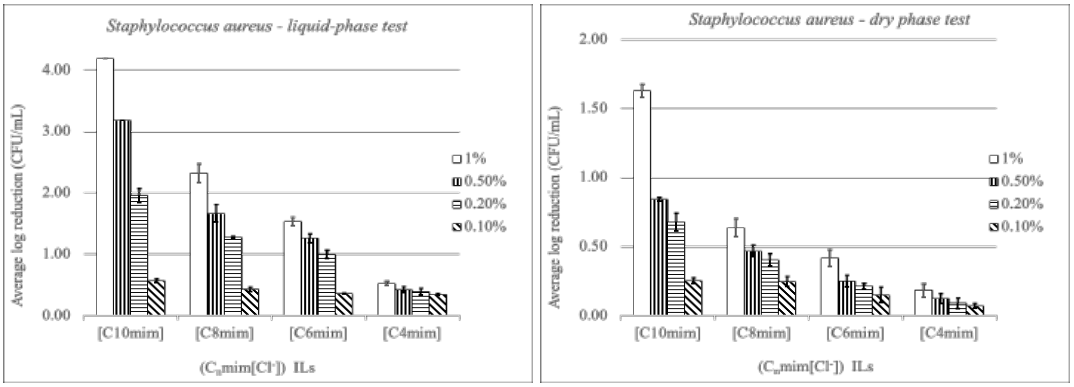

Fig. (1) liquid-phase bactericidal activity (2) dry-phase bactericidal activity of (CnMIM[Cl-]) of varying alkyl chain lengths on *Staphylococcus aureus* bacteria.

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CBF - D3 - P06
What lipid composition best reproduces the biophysical properties of fungal membranes?

Obed Obeng-Gyasi[1], Jyothsna Karman[1], Evelyne Deplazes[1]
[1]School of Chemistry and Molecular Bioscience, University of Queensland, Brisbane, Australia

Current antifungal drugs lack specificity and selectivity, causing host toxicity, and with the current increasing resistance, there is an urgent need for safer and effective options. Fungal plasma membrane and cell wall components differ from those of other eukaryotes, providing suitable targets for drugs. Lipid vesicles provide a useful model system to understand drug-membrane interactions, where lipid composition and environmental factors can be controlled, but model membranes are only useful if they capture the properties of the cellular membrane.
In this project, we investigate the effects of lipid composition on surface charge and fluidity of vesicles aimed at mimicking fungal membranes. For this, we compare simple lipid vesicles, complex lipid vesicles, and lipid extract vesicles (LEVs) from fungal cells. As expected, ergosterol reduces the fluidity of vesicles composed of zwitterionic phosphatidylcholine lipids (POPC). Interestingly, adding phosphatidylethanolamine lipids (POPE), a zwitterionic lipid sharing the same lipid tail saturation as POPC, significantly reduces the fluidity of PC-ergo vesicles, with a change comparable to that of ergosterol. The addition of anionic lipids further reduces fluidity, indicating that headgroups are as relevant to fluidity as tail saturation or the presence of sterols. A combination of ergosterol, POPE and anionic lipids is required to mimic the fluidity of LEVs. As fungal membranes are enriched in anionic lipids, LEVs showed large negative zeta potentials, and at least 40mol% anionic lipids are required to mimic their surface charge. Surprisingly, fungal cells show much lower zeta potential, indicating that the cell wall shields the negatively charged membrane surface.

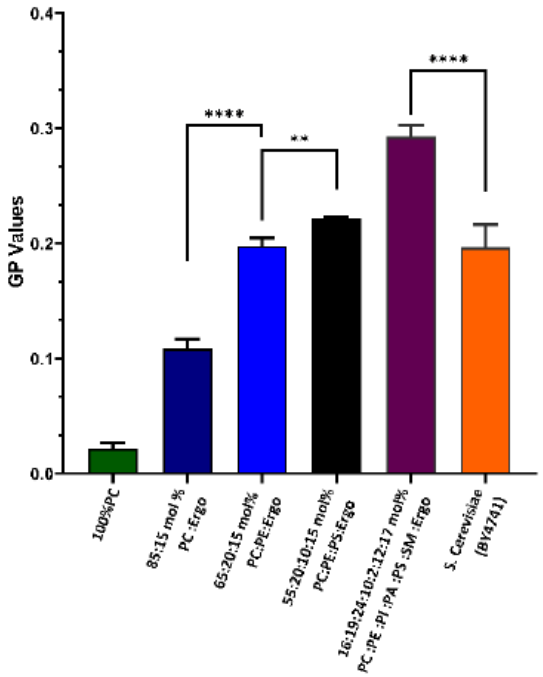

Fig. 1. Generalised Polarisation (G.P.) of the vesicles. Bar plots show Mean ± SEM for at least three replicates. Asterisks indicate **P<0.005, and ****P<0.0001

CBF - D4 - P01
High-resolution mass spectrometry: Unlocking the chemical complexity of xylem sap

Maria Assunta Crescenzi[1,2], Zeinab Hamouche[2,3], Vincenzo Verrastro[3], Erica Tinelli[2], Daniele Cornara[2], Paola Montoro[1]
[1]Dept. of Pharmacy, University of the Study of Salerno, Italy; [2]Dept. of Soil, Plant and Food Science (DiSSPA), University of Bari, Italy; [3]CIHEAM-Bari, Italy

Mass spectrometry (MS) is a powerful analytical tool for the comprehensive characterization of xylem sap, offering exceptional sensitivity, specificity, and the ability to detect a broad spectrum of metabolites, from primary to secondary metabolism-related compounds. High-resolution MS (HR-MS) further enhances these capabilities, enabling precise mass measurements, robust molecular formula assignment, structural elucidation, and the identification of metabolites in biological matrices even at trace concentrations [1]. Untargeted HR-MS approaches facilitate the discovery of novel biomarkers and metabolic patterns that are otherwise inaccessible with conventional techniques. Applications of this technology include the investigation of plant responses to abiotic stress, the characterization of the molecule(s) underlying plant–herbivore interaction, and the evaluation of environmental drivers shaping xylem chemistry [2]. A particularly innovative application is the study of xylem sap composition in relation to host plant acceptance and colonization by xylem-sap feeding insects, such as *Philaenus spumarius* (also known as the meadow spittlebug), the main European vector of *Xylella fastidiosa* ST53 to olive plants [3]. In the present study, xylem sap samples from several *Olea europaea* varieties were profiled using an untargeted metabolomics workflow to identify metabolites potentially associated with acceptance or rejection by *P. spumarius*. The metabolites detected predominantly belong to the chemical classes of organic acids, amino acids, sugars, terpenes, and phenolic compounds, which were subsequently selected for targeted quantitative analysis. Collectively, this study represents the first comprehensive characterization of xylem sap metabolites mediating spittlebug-olive interaction, and successive pathogen transmission. Additionally, the results lay the groundwork for the selection of potentially resistant germplasm and the development of agronomic strategies aimed at reducing host plant suitability for the vector, thereby contributing to the containment of pathogen spread.

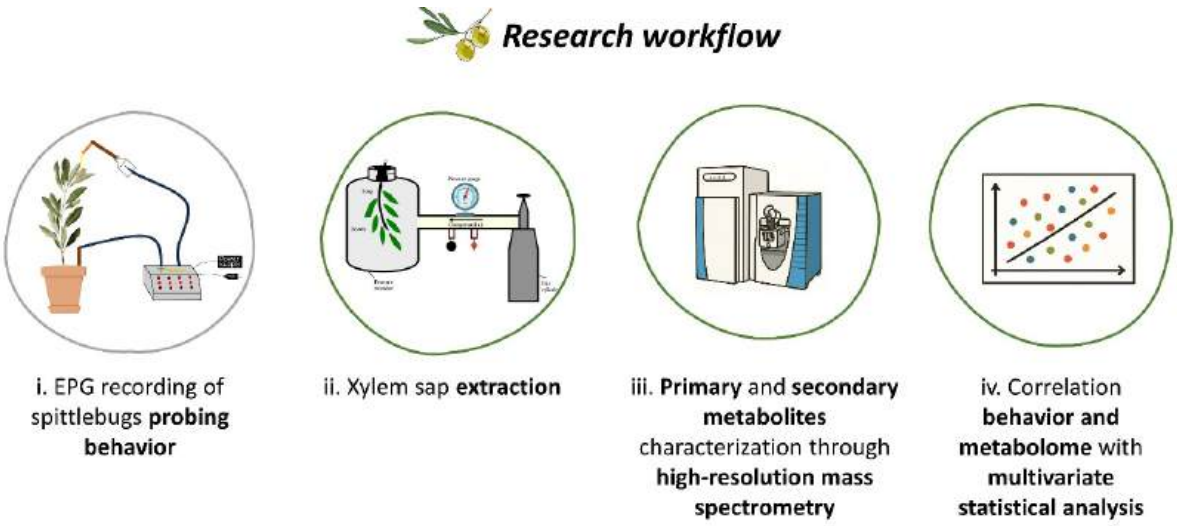

Fig. 1. Experimental workflow illustrating EPG-based recording of spittlebug feeding behaviour, xylem sap extraction, high-resolution mass spectrometry–based metabolomic profiling, and multivariate analysis integrating behavioural and chemical data.

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CBF - D4 - P02

Stability meets mobility: *N*-heterocyclic carbene-based tethers for functional biomimetic membranes

Lavinia Klement[1], Martin Waxmann[1], Dorian Bader[1], Nicoletta Ditaranto[2,3], Brigitte Holzer[1]
[1]Institute of Applied Synthetic Chemistry, TU Wien, Austria; [2]Dipartimento di Chimica Università degli Studi di Bari Aldo Moro, Italy; [3]CSGI (Center for Colloid and Surface Science) Bari Unit, Italy

Biological membranes exhibit extraordinary structural and functional complexity, making simplified model systems essential for understanding individual membrane components and processes. Tethered bilayer lipid membranes (tBLMs) provide a powerful platform for such studies. However, conventional thiol-based anchors have a limited lipid mobility and stability under ambient conditions.[1–3]

Here, we present the design, synthesis and characterization of novel *N*-heterocyclic carbene (NHC)-based tethered bilayer lipid membranes assembled in gold substrate as stable alternative to currently used systems with an optimized surface density and increased mobility.[4]

Self-assembled monolayer (SAM) formation was achieved under mild conditions[5] using triflate NHC precursors and surface density was systematically tuned through a variation of *N,N*-substituents.[6] Successful SAM formation was confirmed by contact angle measurements, cyclic voltammetry and X-ray photoelectron spectroscopy (XPS).

To assess the applicability of NHC-based SAMs for membrane model systems, lipid bilayers were formed using vesicle fusion with commercially available lipids. Electrochemical impedance spectroscopy (EIS) was employed to test bilayer formation and functional performance, and results were compared to conventional thiol-tethered systems.

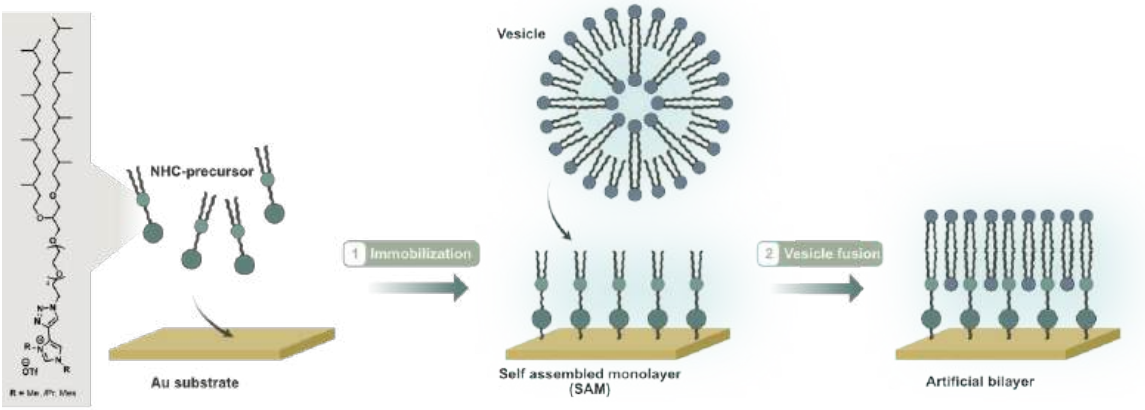

Fig. 1. Formation of (1) a self-assembled monolayer (SAM) using NHC-triflate salt precursors and (2) an artificial bilayer using vesicle fusion

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CBF - D4 - P03

Effect of Noscapine Hydrochloride on the near-infrared optical properties of Indocyanine Green

Ankita Borah[1], Snigdha Singh[1,2]

[1]Dept. of Chemistry, University of Delhi, India; [2]Institute for Nanomedical Sciences (INMS), University of Delhi, India

Indocyanine Green (ICG) is an FDA-approved near-infrared fluorophore widely utilized in biomedical imaging and photothermal therapy. However, its clinical applicability is limited by poor stability, rapid degradation, and concentration dependent aggregation. In this study, we report for the first time the role of Noscapine hydrochloride (Np·HCl), a benzyl isoquinoline alkaloid with established anticancer properties, in modulating the optical and therapeutic characteristics of ICG through controlled aggregation. Spectroscopic investigations revealed that Np·HCl promotes intermolecular aggregation of ICG at micromolar concentrations. Absorption studies demonstrated concentration dependent spectral shifts and intensity variations, indicating the coexistence of H- and J-type aggregates. Gaussian deconvolution of absorption spectra confirmed redistribution of monomer and aggregate populations, with the appearance of new near-infrared band (~835 nm) signifying J-aggregate formation. Fluorescence measurements showed progressive quenching of ICG emission with increasing Np·HCl concentration, supported by Stern Volmer analysis suggesting combined static and dynamic quenching mechanisms. Stability studies demonstrated enhanced resistance of ICG towards photodegradation and long-term storage upon complexation with Np·HCl. Zeta potential and dynamic light scattering analysis confirmed the formation of stable nano-aggregates, attributed to electrostatic interactions between protonated noscapine and sulfonate groups of ICG, facilitating π-π stacking of chromophores. Further, *in vitro* cytotoxicity studies against H1299 lung adenocarcinoma cells showed dose-dependent anticancer activity. The ICG:Np·HCl combination exhibited significantly enhanced cytotoxicity with IC_{50} values of 354.4 μM and 165.8 μM for ICG and Np·HCl, respectively, demonstrating synergistic therapeutic effects. These findings highlight a novel dye-drug assembly strategy that improves both optical stability and anticancer efficacy, offering potential applications in combined chemo-photothermal therapy.

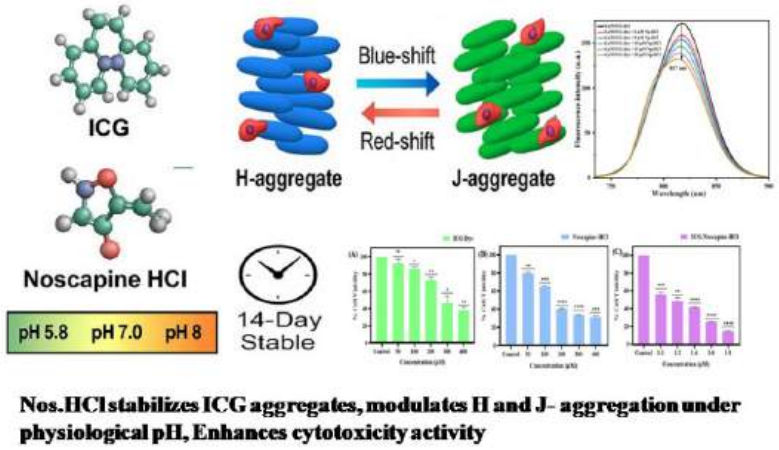

Fig. 1: Graphical abstract

Borah A. (UGC ID: 231620214515) is thankful to UGC for providing financial assistance. S.S and A.B are thankful to Dept. of Chemistry and Institute for Nanomedical Sciences (INMS), University of Delhi for infrastructure. All authors are thankful to USIC for instrumentation facilities. S.S. is also thankful to IOE for providing financial assistance. (Ref. No./IoE/2024-25/12/FRP).

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CBF - D4 - P04

Lead-silica interactions in food additive E551: Concentration-dependent effects on surface charge and colloidal stability

Beatriz Pinto[1], Filipa Bastos[2,3,4,5], João P. Teixeira[2,3,4], Ana T. Reis[2,3,4], Cláudia B. Lopes[1]
[1]Dept. of Chemistry and Aveiro Institute of Materials (CICECO), University of Aveiro, Portugal; [2]EPIUnit—Instituto de Saúde Pública, Universidade do Porto, Portugal; [3]Laboratório para a Investigação Integrativa e Translacional em Saúde Populacional (ITR), Portugal; [4]Environmental Health Dept., National Institute of Health,Portugal; [5]Instituto de Ciências Biomédicas Abel Salazar (ICBAS), Universidade do Porto, Portugal

With advances in nanotechnology, the use of nanomaterial-based food additives has increased, improving food quality and functionality. However, this trend also raises concerns about potential interactions between these additives and co-occurring chemical contaminants in food and water. Such interactions may modify properties, including particle size, structure, morphology and surface characteristics (Figure 1), and therefore influence the nanoparticles (NPs) behaviour and bioavailability.

In this study, developed within the MixIng-Tox project (2022.03491.PTDC), we investigated how lead (Pb) affects the physicochemical properties of the silica-based food additive E551. Four experimental scenarios were tested by combining two E551 concentrations (300 and 3000 mg·kg^{-1}) with two Pb^{2+} concentrations (1.0 and 3.0 mg·kg^{-1}).

Stable suspensions of the silica-based food additive E551were prepared using the Nanogenotox procedure and characterised using dynamic light scattering (DLS), zeta potential measurements and electron microscopy. At low E551 concentration (300 mg·kg^{-1}), Pb^{2+} decreased the magnitude of the zeta potential, consistent with partial charge neutralisation, while hydrodynamic size and polydispersity index (PdI) showed no clear concentration-dependent trend. In contrast, at high E551 concentration (3000 mg·kg^{-1}), the zeta potential remained strongly negative and was not measurably affected by Pb^{2+}. This behaviour mirrors our previous observations for Cd^{2+}.

Overall, our results reveal a concentration-dependent interplay between E551 and Pb^{2+} governed primarily by surface charge and ionic interactions. Mechanistic understanding of these processes is essential for realistic assessments of nanomaterial stability and behaviour in complex food matrices, supporting more accurate evaluations of dietary exposure and risk arising from both nanomaterial additives and co-existing chemical contaminants.

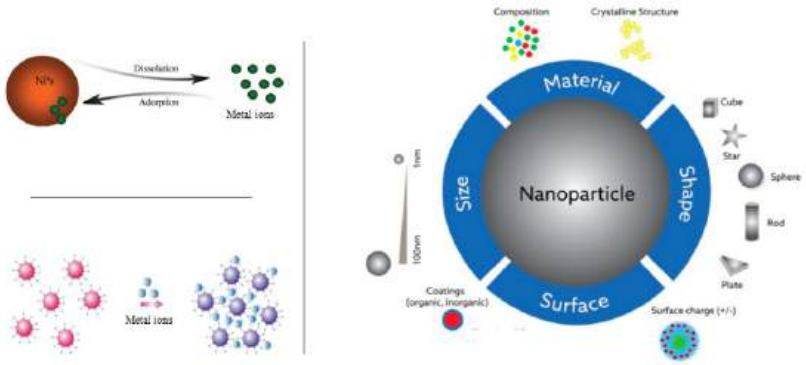

Fig.1. Possible interactions between metal ions and nanoparticles, and key NPs properties.

This work was supported by Fundação para a Ciência e Tecnologia (FCT), I.P., through MixIng-Tox (2022.03491.PTDC; DOI: 10.54499/2022.03491.PTDC) and the projects UIDB/04750/2020 (DOI: 10.54499/UIDB/04750/2020), LA/P/0064/2020 (DOI: 10.54499/LA/P/0064/2020), UID/50011/2025 (DOI: 10.54499/UID/50011/2025) and LA/P/0006/2020 (DOI: 10.54499/LA/P/0006/2020), financed by national funds via FCT/MCTES (PIDDAC). A.T. Reis acknowledges FCT support via MixIng-Tox. C.B. Lopes acknowledges FCT support through contract 10.54499/2021.03739.CEECIND/CP1659/CT002. F. Bastos acknowledges FCT PhD grant 2024.01615.BDANA.

CBF - D4 - P05
Effect of drying methods and pretreatments on the carbohydrate profile of Pingo de Mel figs

Ramla Khiari[1], Elisabete Coelho[1], Joana Barros[1], Manuel A. Coimbra[1]
[1]LAQV-REQUIMTE, Dept. of Chemistry, University of Aveiro, Aveiro, Portugal

Figs are widely consumed globally due to their appealing taste and high sugar content, which provides a valuable energy source [1]. While figs are traditionally dried whole, pretreatments applied before dehydration not only accelerate the drying process but also enhance product quality [2]. Despite this knowledge, no previous studies have examined how pretreatment affects the carbohydrate profile of figs. This study investigated the influence of different drying conditions on carbohydrate composition and extractability in the "Pingo de Mel" fig variety.
"Pingo de Mel" figs were dried in a solar dryer at 50 °C using three methods: whole figs without pretreatment, blanched figs in hot water, and halved figs. Sequential extraction with ethanol and water (cold and hot) yielded three soluble fractions (snAIR, CWE, and HWE) and one insoluble residue (WIR). Commercial sun-dried figs from local farmers served as controls. Carbohydrate profiles were characterized using Gas Chromatography coupled with Flame Ionization Detection (GC-FID), while uronic acids were quantified spectrophotometrically.
Results showed that although all samples had similar total sugar content, drying conditions significantly affected the sugar profile, particularly increasing solubilized pectic polysaccharide levels. Uronic acid was the major carbohydrate, reaching 82% and 70% in the CWE of halved and blanched figs, respectively, an increase by more than 1.2-fold over whole figs (62%). These fractions along with the HWE exhibited increased arabinose, xylose, and mannose levels. The elevation of arabinose and xylose suggests enhanced solubilization of pectic polysaccharides with arabinan side chains. The WIR fraction contained glucose, xylose, galactose, and arabinose, indicating the presence of xyloglucans which were also detected in higher amounts in pretreated samples.
Overall, pretreatment influenced the carbohydrate composition of "Pingo de Mel" figs by favoring the solubilization of pectic polysaccharide, suggesting its potential application for improving the extractability of these cell wall polysaccharides.

Keywords: Fig, carbohydrates, polysaccharides, pretreatment, drying.

Acknowledgements: The authors are grateful for the financial support from project PrOSFig that is part of the HORIZON-WIDERA-2023-TALENTS-02-01 supported by the European Union, Grant Agreement ID: 101180656. This work is also based upon work from InovFarmer.MED - Improving Mediterranean supply chain through innovative agro-food business to strengthen small-scale farmers competitiveness, using prickly pear and fig as case study (PRIMA/0006/2021) through FCT. The authors acknowledge the financial support through LAQV/REQUIMTE, UID/50006 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos, within the PT2020 Partnership Agreement. The authors acknowledge the financial support through LAQV/REQUIMTE, UID/50006 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos, within the PT2020 Partnership Agreement. The authors thanks Pr. Dulcinea Wessel and Dr. Cláudia M.B. Neves from the IPV, for their collaboration in providingof fig samples. Elisabete Coelho thanks FCT for the research contracts (DL 57/2016/CP1482/CT0038, 2023.08855.CEECIND).

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CBF - D4 - P06

The effect of processing technology on the content of acrylamide, amino acids, and reactive dicarbonyl compounds formed during bread baking

Małgorzata Starowicz[1], Joanna Honke[1], Kristína Kukurová[2], Maria Kopuncova[2], Zuzana Ciesarová[2], Małgorzata Wronkowska[1]

[1]InLife Institute of Animal Reproduction and Food Research, Poland; [2]NPPC, Slovakia

Thermal processing and long-term storage of food initiate complex chemical reactions between carbonyl groups of reducing sugars and amino groups of amino acids, peptides, and proteins. This set of reactions, known as the Maillard reaction, is responsible for desirable flavor, aroma, and color formation, but also for the generation of potentially harmful compounds such as acrylamide and reactive dicarbonyls, including methylglyoxal (MGO) and glyoxal (GO). Free asparagine is recognized as a key precursor in acrylamide formation, and its concentration in cereal raw materials may significantly influence acrylamide levels in processed foods.

The present study aimed to evaluate the content of amino acids and Maillard reaction products in model bakery products obtained from two oat varieties (spring and winter) and to determine the effect of baking parameters on their formation. Breads were prepared under two baking conditions (200°C/90 min and 180°C/120 min). The content of amino acids (Asn, Asp, Gln, Glu), acrylamide, and reactive dicarbonyls (MGO, GO) was determined using previously developed HPLC and LC-MS methods.

Spring oat grain contained approximately twice the level of the analyzed amino acids compared to winter oat; however, this difference was not reflected in the final bread products. Baking parameters significantly affected acrylamide and carbonyl compound formation. Lower temperature combined with extended baking time reduced their levels, whereas increasing temperature and time resulted in a twofold rise in acrylamide content and a fourfold increase after parameter modification in breads from both oat varieties. No significant varietal effect on the analyzed compounds was observed.

The results confirm that time and temperature are critical determinants of Maillard reaction product formation in fresh bread, while further characterization of oat varieties may support the development of improved cereal-based products.

Acknowledgments: This contribution was supported by COST Action CA21149 (Reducing acrylamide exposure of consumers by a cereals supply-chain approach targeting asparagine (ACRYRED); https://acryred.eu/)

CBF - D4 - P07

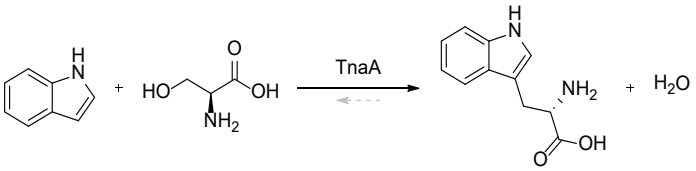
Mining for novel tryptophanase A: extremophilic organisms *Ardenticatena maritima* and *Haloarcula japonica* as alternative to *E. Coli* in the synthesis of tryptophan analogues

Fatemeh Aziziyan[1], Evelyn Sgroi[1], Francesca Paradisi[1]
[1]Dept. of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Switzerland

L-Tryptophan is a key amino acid with significant roles in both biological systems and pharmaceutical industries. Beyond its natural role in cellular metabolism, L-tryptophan derivatives and other non-canonical amino acids (ncAAs) are increasingly valued in medicinal chemistry and synthetic biology, contributing to the design of chemical probes and pharmaceutical scaffolds.[1,2] The biosynthesis of L-tryptophan is classically mediated by the heterodimeric tryptophan synthase (TrpS)[3], however, in *Escherichia coli* strains, it has also been well-documented that L-tryptophan can be synthesized under high concentrations of L-serine via tryptophanase A (*Ec*TnaA), an enzyme typically involved in L-tryptophan catabolism (Figure 1).[4]

Scheme 1. Biosynthesis of L-tryptophan from indole and L-serine.

This research focuses on the characterization of two novel TnaA enzymes: *Am*TnaA from the thermophilic organism *Ardenticatena maritima*[5] and *Hj*TnaA from the halophilic organism *Haloarcula japonica*.[6] Owing to their resilience under harsh physicochemical conditions, these enzymes represent promising biocatalytic tools for challenging synthetic applications, and the exploration of their substrate scope further highlights their potential for sustainable production of tryptophan derivatives and pharmaceuticals.



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CBF - D4 - P08

Implementation and optimization of automated computer processing tools for a bi-instrumental systematic toxicological analysis strategy using HPLC-DAD and GC-MS

Khaled Sobhi, Mohamed Redha Difallah, Houssem Ouzouigh
Toxicology Laboratory, Army Central Hospital, Algiers, Algeria

To modernize the laboratory's bi-instrumental Systematic Toxicological Analysis (STA) strategy, automated post-analytical interpretation tools were implemented and optimized to enhance performance, reduce time, and improve efficiency in identifying unknown toxic substances in biological samples.

Two analytical techniques, HPLC-DAD and GC-MS, were employed alongside acetylation and silylation derivatization methods. For post-analytical interpretation, Empower 2 software with the "Toxicol" library was used for HPLC-DAD data, while AMDIS combined with NIST-MS-Search and custom libraries (MPW5e, Forensic_Toxicology_V2, W11N17) supported GC-MS analysis. Calibration for Retention Indices (RI) was applied to AMDIS.

Three sets of processing parameters were defined for each chromatographic method and evaluated using chromatograms from mixtures of analytical standards. Data compilation and visualization were performed using Microsoft Excel, and MS reference libraries were modified with OpenChrom and Lib2NIST.

Empower 2's library contains 1,087 UV spectra, AMDIS uses a custom library of 11,103 MS spectra, and NIST-MS-Search accesses over 1.25 million reference MS spectra. Calibration of AMDIS for RI was successful. Detected compounds were organized by instrument and derivatization method.

Performance evaluation considered the number of compounds identified and the time required for interpretation.

Manual interpretation by an experienced toxicologist takes 30 to 40 minutes, whereas Empower 2 reduces this to 55 seconds and AMDIS to 2 minutes 30 seconds. This significant time saving facilitates routine and emergency toxicological analyses. Despite automation, expert review remains essential to ensure accuracy and reliability.

The integration of optimized automated tools for bi-instrumental STA notably enhances laboratory efficiency, enabling rapid and reliable toxicological identification while maintaining critical expert oversight.

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CBF - D4 - P09
Membrane organoid chips for programmable growth of stem cells

Evelin Schäfer[1], C. You[1], L. Tveriakhina[1], M. Steinhart[1]
[1]Osnabrück University, Germany

Organoid research faces challenges in controlling microenvironmental factors and modelling complex tissue interactions. Porous membrane-based organoid chips may overcome these limitations as they potentially provide a defined 3D environment with adjustable signal gradients across a semipermeable nanoporous membrane, enabling precise control of organoid culture conditions. This approach is expected to improve organoid homogeneity and enable statistically reliable high-throughput screening. Porous membrane-based organoid chips are, therefore, a promising tool for the further development of basic organoid research and for applications in drug discovery. [1, 2] Here, we present initial results regarding the development of topographically patterned membrane-based organoid chips consisting of the block copolymer polystyrene-block-poly(vinylpyridine) (PS-*b*-P2VP). The chips' hierarchical architecture comprises topographical niches generated by replication moulding to accommodate stem cells, cell clusters and organoids as well as continuous mesopore systems generated by selective swelling-induced pore formation [3] for the transport of medium to the niche bottoms. The fabrication of spongy mesoporous PS-*b*-P2VP monoliths containing mesopore systems as well as topographic niches and subsequent cultivation of different cells as well as an initial differentiation of induced pluripotent stem cells into hepatoblast bodies is reported.

The authors thank the German Research Foundation (RTG 2900 nanomaterials@biomembranes, project number 501879556) for funding.

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CBF - D4 - P10
Proteomics in the multi-omics era: A key to safer drugs and deeper disease insights

Andrzej Gawor, Ewa Bulska
University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Poland

Proteomics plays a pivotal role within the broader omics framework by bridging genetic and transcript-level information with functional outcomes at the level of proteins. Since proteins act as the main drivers of cellular activity, proteomic analyses offer insights into biological processes and drug-induced effects that cannot be completely resolved through genomics or transcriptomics alone. When combined with other omics layers such as transcriptomics and metabolomics, proteomics contributes to a comprehensive, system-wide understanding of biological responses relevant to disease and pharmacological interventions.
In this presentation, we emphasize the importance of mass spectrometry-based proteomics as a foundational component of multi-omics approaches in biomedical research and drug safety evaluation. Proteomics enhances these integrative strategies by enabling detailed characterization of protein expression changes, post-translational modifications, and molecular alterations resulting from chemical or pharmaceutical exposure.
To illustrate the breadth of this approach, we present selected case studies demonstrating its application across different research contexts. These include investigations of drug-related protein modifications associated with fluorinated compounds, studies of protein expression changes linked to disease states, and analyses of inflammatory signaling pathways in skin disorders such as psoriasis. Collectively, these examples demonstrate how proteomics can provide mechanistic insights into both therapeutic actions and adverse drug effects.
By establishing proteomics as a central component of integrated omics workflows, this work highlights its essential role in advancing modern pharmacology and translational science. The integration of diverse omics datasets improves mechanistic understanding, facilitates biomarker identification, and strengthens the predictive accuracy of safety assessments. Ongoing developments in analytical methodologies and data integration are expected to further expand the impact of multi-omics strategies in the design of safer and more effective therapeutic solutions.

CBF - D4 - P11
PATHFOOD: From soil to health - Analytical chemistry driving selenium-enriched functional foods

Ewa Bulska
University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Poland

The development of functional foods enriched with essential micronutrients represents a key challenge at the interface of chemistry, biology, and food science. Selenium (Se), an essential trace element with well-documented health benefits, plays a crucial role in human metabolism, yet its dietary intake remains insufficient in many regions. The PATHFOOD project, coordinated by the University of Warsaw, addresses this issue through an integrated approach combining analytical chemistry, plant science, and food technology.
This study focuses on the design of a sustainable selenium-enriched functional food chain, from biofortification of crops to final product development. Innovative cultivation strategies are applied to enhance selenium uptake in plants while minimizing environmental impact. Subsequent processing methods are optimized to preserve selenium content and bioavailability.
A central aspect of the project is the application of advanced analytical techniques, including inductively coupled plasma mass spectrometry (ICP-MS), for precise quantification and speciation analysis of selenium in plant matrices and food products. These methods enable the assessment of selenium distribution, bioavailability, and safety, ensuring compliance with regulatory standards.
The results demonstrate that combining biofortification strategies with state-of-the-art analytical tools allows for effective monitoring and control of selenium throughout the food production chain. This integrated approach supports the development of safe, high-quality functional foods and contributes to improved public health outcomes.
The PATHFOOD initiative exemplifies how analytical chemistry can bridge the gap between biological systems and food science, fostering sustainable innovation through international collaboration and knowledge exchange.

Funding: This research was funded by the European Union under the Horizon Europe research and innovation programme (2021–2027), within the PATHFOOD project (Creating a Functional and Sustainable Food Chain: A Path to Climate Neutrality and Improved Health in the EU), grant agreement No. 101160011.

CBF - D4 - P12
Identification of isothiocyanate-hydrolyase candidate proteins by in-silico modelling

Nicolas Proksch[1], Katja Witzel[2], Laura Lamelas Penas[3], Franziska S. Hanschen[1,4]
[1]Phytonutrient Management, Leibniz Institute of Vegetable and Ornamental Crops (IGZ) e.V., Germany; [2]Science Support Platform, Leibniz Institute of Vegetable and Ornamental Crops (IGZ) e.V., Germany;[3]Temperature Sensing in Plants, Leibniz Institute of Vegetable and Ornamental Crops (IGZ) e.V., Germany; [4]Phytonutrient Management, Institute of Food Technology and Food Chemistry, Technische Universität Berlin, Germany

Glucosinolate-derived isothiocyanates (ITC) are well known for their health promoting properties, such as anticarcinogenic effects.[1] While ITC also serve as key plant defense compounds, a recent study by Andernach et al.[2] suggested the presence of a plant-endogenous ITC hydrolase (ITCase) in Brassica oleracea. ITCase-mediated breakdown of ITC to amines can result in the loss of these beneficial compounds and to the accumulation of amines whose bioactive properties remain poorly characterized. As the responsible enzyme is not yet identified, this study aims to identify possible candidate proteins by in silico modelling using Boltz-2[3], [4] after protein isolation for further verification as recombinant proteins.
Proteins were extracted from lyophilized Brussels sprouts by sonication after two wash outs, followed by ammonium sulfate precipitation and preparative size-exclusion FPLC. ITCase activity was determined by incubating samples with 3-butenyl ITC and quantifying the resulting amine by LC-MS/MS MRM.[2] Active fractions were analyzed by bottom-up proteomics via nanoLC-HRMS and additionally field asymmetric ion mobility spectrometry (FAIMS) was used due to detergent-induced signal suppression. Annotated proteins with a minimum coverage of 10% and two unique peptides were used for co-folding with 3-butenyl ITC and water as substrates and Zn2+ as a cofactor using Boltz-2.[3], [4]
Of four fractions isolated by preparative size-exclusion FPLC, only for peak 2, which showed the highest absorbance at 280 nm, an ITCase activity of 15% relative to the crude extract was determined, with a purification factor of 5.5. 86 proteins were annotated by bottom-up proteomics by combining nanoLC-HRMS and FAIMS. To further narrow down possible ITCase candidates, in-silico modelling was performed for the annotated proteins. For 14 out of 86 proteins the predicted 3D structures contained promising active centers consisting of Zn2+ coordinated mainly by histidine residues and the substrates located near the metal ion, while achieving acceptable to good quality parameters. These 14 candidate proteins represent potential plant-endogenous ITCases in B. oleracea and will be prioritized for recombinant expression and functional validation.

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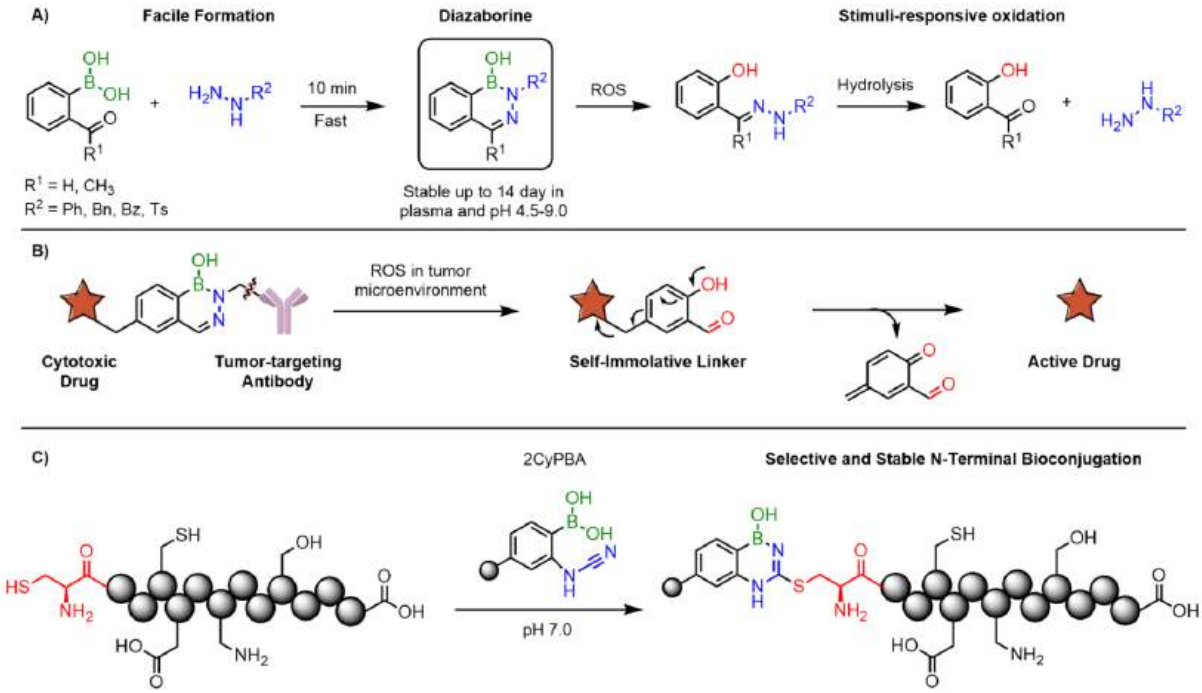
CBF - D4 - P13

Click! Bioconjugate! Release!: A unified diazaborine platform for stimuli-responsive therapeutics

João P.M. António[1], Joana Inês Carvalho[1], Ana S. André[2], Joana N.R. Dias[2], Sandra I. Aguiar[2], Hélio Faustino[1], Ricardo M.R.M. Lopes[1], Luis F. Veiros[3], Gonçalo J.L. Bernardes[4,5], Rita Padanha[1], Rafaela A.N. Cavadas[1], Pedro Merino[6], Frederico A. da Silva[2], Pedro M.P. Gois[1]

[1]Research Institute for Medicines (iMed.ULisboa) Faculdade de Farmácia, Universidade de Lisboa; [2]Faculdade de Medicina Veterinária, Universidade de Lisboa; [3]Instituto Superior Técnico, Universidade de Lisboa; [4]Faculdade de Medicina, Universidade de Lisboa; [5]Dept. of Chemistry, University of Cambridge. [6]Universidad de Zaragoza,Spain

Antibody-drug conjugates (ADCs) are among the most promising therapeutic strategies in oncology. Central to their success is the linker, since it must remain stable in circulation but release the payload selectively within cancer cells. We recently developed diazaborines (DABs) as a novel ROS-responsive motif, exploiting the oxidative microenvironment of tumors to enable the design of a first-in-class ROS-activatable ADC. DABs form rapidly under bioorthogonal conditions (pH 7.4, 10 min), display excellent stability in buffer and plasma (pH 4.5–9.0), and are readily oxidized by H_2O_2 ($t_1/_2$ = 15 min with 100 equiv.). A DAB-based self-immolative linker was incorporated into a homogeneous ADC bearing SN-38 and a B-cell lymphoma-targeting antibody, yielding potent activity (IC_{50} = 54.1 nM) and high selectivity (>100 μM in T-cell lymphoma). To expand the utility of this chemistry, we developed a site-selective strategy for installing DABs directly onto peptides via chemoselective cysteine alkylation. Using (2-cyanamidophenyl)boronic acids (2CyPBAs), DABs can be formed *in situ* through selective reaction with *N*-terminal cysteines, guided by an intramolecular B–N bond. The reaction proceeds under mild, aqueous conditions, shows high conversion across diverse peptide sequences, and exhibits strict selectivity over internal cysteines. This method gives new life to DAB chemistry by enabling its direct incorporation without the need for auxiliary bioconjugation handles and opening new opportunities for targeted therapeutics and functional bioconjugates.



Acknowledgements: We thank the FCT for financial support (2022.06817.CEECIND and 2024.16254.PEX)

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Posters

Catalyzing New Chemistry Solutions (CCS)

CCS - D1 - P01
The controlled transfer hydrogenation of muconates using Ru based catalysis

Lisa De Vriendt[1], Ibrahim Khalil[2], Matthew Hickson[1], Bert Sels[1], Michiel Dusselier[1]
[1]KU Leuven (CSCE), Belgium; [2]Lyon 1(Ircelyon), France

Muconic acid (MA) is a potentially biobased compound that can serve as a platform chemical towards high value monomers (adipic acid, terephthalic acid, caprolactam, ...).[1–3] Adipic acid (AA) can be synthesized by the hydrogenation of the carbon bonds in MA. When selectively hydrogenating MA, hexenedioic acid (HDA), a monounsaturated compound with four isomers, can be obtained. This compound can serve as an alternative for AA in nylon-6,6, enabling further property tuning of the polymer by inserting functional groups.[4] Electrocatalytic routes towards the t-3-isomer exist, but catalytic hydrogenations towards HDA are very limited.[5] This work shows the first monohydrogenation of MA towards HDA without AA formation (Figure 1).[6] Catalytic transfer hydrogenations with ethanol as hydrogen source are performed using ruthenium complexes as catalysts.
Seven Ru-complexes were tested for the monohydrogenation of *trans, trans*-diethyl muconate (*tt*DEM), of which only $RuCl_3.3H_2O$ showed no further hydrogenation towards diethyl adipate (DEA). Isotopically labelled experiments showed a 2,5-hydrogenation followed by rapid isomerization towards the *t*-2-isomer takes place. The hydrogenation mechanism was also investigated via isotopic labelling, showing a monohydride type isomerization and hydrogenation. Acid substrates were tested as well, but were outperformed by the esters, because of improved solubility and absence of lactonization in case of the esters.[6] More recent work is focused on working towards a reusable heterogeneous catalyst for this reaction. Ruthenium loaded zeolites are showing promising results. Different supports, loading methods, loading amounts, activation protocols and reaction conditions were investigated.

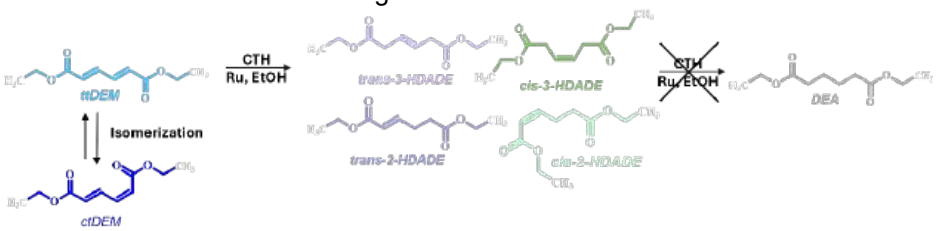

Fig. 1. Overview of the CTH of cis,trans and trans,trans-diethyl muconates (ctDEM and ttDEM) towards HDADE (hexenedioic acid diethyl ester, 4 isomers), with the goal to avoid the full hydrogenation towards diethyl adipate (DEA).

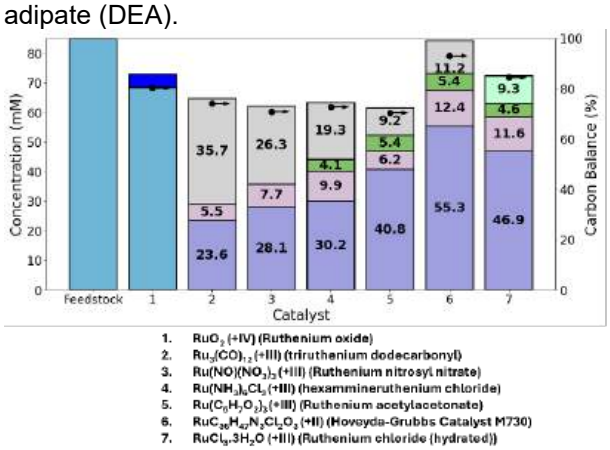

Fig. 2. Results of the catalytic screening of different Ru precursors (RuO_2, $Ru_3(CO)_{12}$, $Ru(NO)(NO_3)_3$, $Ru(NH_3)_6Cl_3$, $Ru(C_5H_7O_2)_3$, $RuC_{36}H_{47}N_3Cl_2O_3$ and $RuCl_3.3H_2O$ in the transfer hydrogenation of ttDEM (diethyl muconate). Reaction conditions: 85 mM ttDEM, 5 mL EtOH, 175 °C, Ru/MA (mol/mol) = 1/50, 14 bar N2, 5 hours. Colors correspond to figure 1.

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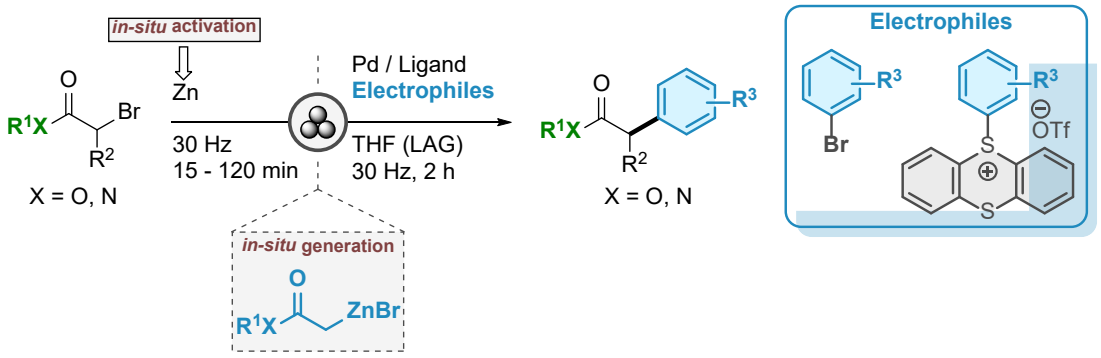
CCS - D1 - P02
Mechanochemical utilization of Reformatsky Zn-enolates in cross-coupling reactions

Tomáš Čarný[1], Dominika Mravcová[1], Barbora Steinhüblová[1], Radovan Šebesta[1]
[1]Dept. of Organic Chemistry, Faculty of Natural Sciences, Comenius University Bratislava, Slovak Republic

Although many cross-coupling reactions have become an almost routine part of the organic synthesis, significant challenges remain, and more practical or mild reaction conditions are highly desirable. The primary disadvantages are sensitivity to moisture and oxygen, high reactivity or requirement to operate at low temperatures. In the past decades, transition-metal-catalyzed α-arylations of carbonyl compounds have proved to be a useful strategy for the synthesis of α-aryl esters. However, the use of strong bases and difficult handling of some organometallic compounds is a major disadvantage. On the other hand, Reformatsky Zn-enolates are valuable synthetic reagents, that can overcome these issues, however their sensitivity to moisture may represent certain limitations during the preparation and isolation.[1,2] To overcome these challenges, we have developed a mechanochemical Pd-catalyzed cross-coupling of *in-situ* generated Reformatsky Zn-enolates. This operationally simple procedure delivered 21 α-arylated products up to 95% yield using an affordable catalytic system and commercially affordable aryl bromides. Reactions were carried out under ambient conditions using granulated zinc without its pre-activation. The optimized conditions were applied in a scale-up reaction and in the synthesis of α-arylated esters, amides, and derivatives of natural products.[3] Recently, we developed a new methodology utilizing Reformatsky enolates together with solid thianthrenium salts, that can be used as an unconventional electrophiles suitable for mechanochemical cross-coupling reactions.



This work was supported by the Slovak Research and Development Agency under the Contract APVV-22-0167 and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00024.

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CCS - D1 - P03

Synergistic graphene/CuO coatings by an intermittent spray-coating to enhance the thermal decomposition and performance of ammonium perchlorate

Akbi Hamdane[1]
[1]Ecole Militaire Polytechnique, Algeria

Ammonium perchlorate (AP) is the primary oxidizer in composite solid propellants (CSPs) used in solid rocket motors (SRMs) due to its high oxygen content and stability. However, its high decomposition temperature and activation energy lead to a low decomposition rate and long ignition delay. Moreover, AP's hygroscopicity and tendency to agglomerate can adversely affect combustion and thrust performance[1].

To address these drawbacks, AP is often combined with catalysts, anti-agglomeration agents, and sensitivity reducers. Carbon-based materials, particularly graphene, have shown great promise in enhancing AP's decomposition and reducing hygroscopicity due to their high surface area, hydrophobicity, and excellent conductivity. Yet, pure graphene is difficult to obtain and coat onto AP particles[2].

Graphene oxide (GO), derived easily from graphite and dispersible in various solvents, serves as an effective alternative. GO can be deposited onto AP using simple solution-based techniques such as spray or dip coating. Upon mild heat treatment, GO is reduced to reduced graphene oxide (RGO), restoring conductivity and hydrophobicity while releasing energy (1680 J·g−1) and gas at low temperatures (<200 °C), which can further promote AP decomposition. The removal of oxygen-containing functions (OCFs) from GO by thermal annealing not only enhances its hydrophobicity but also provides an eco-friendly route compared to chemical reduction[3].

This presentation introduces an innovative, scalable method for coating AP with GO via intermittent spray coating and drying. Both AP@GO and AP@CuO@RGO composites were successfully developed using this approach. The coatings preserve the morphology of AP particles while embedding CuO nanoparticles and GO nanosheets uniformly, preventing catalyst agglomeration. Heat treatment of AP@GO at 150 °C effectively transforms the surface from hydrophilic to hydrophobic, reducing hygroscopicity and enhancing the thermal decomposition of AP.

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CCS - D1 - P05

New strategies for catalytic conversion of sugarcane alcohols into valuable chemicals

Mauricio Boscolo[1], Rebeca Casado[1], Isabela Mantelli[1], Eleni, Gomes[1], João Thomeo[1], Gustavo Metzker[1]
[1]Institute of Biosciences, Letters and Exact Sciences (IBILCE), São José do Rio Preto Campus, São Paulo State University (UNESP), Brazil

Sugarcane biorefineries generate two alcohol streams: ethanol and fusel oil (a higher-alcohol mixture). This work reports catalytic strategies to convert these feeds into value-added chemicals using (*i*) La-based perovskites in a fixed-bed reactor for fusel-oil upgrading and (*ii*) Mg/Al hydrotalcite-derived mixed oxides partially substituted with Zn–Ni or Zn–Cu for ethanol conversion[1].

Perovskites ($LaMnO_3$, $LaCoO_3$, $LaNiO_3$) were evaluated (500–600°C, 1–2 h) using fusel oil and fuel oil co-fed with 10% methanol or 10% ethanol. Major products were selected by GC–MS (highest peak areas and spectral match >880). With neat fusel oil at 500°C, product fingerprints depended on the B-site: $LaMnO_3$ favored branched olefins (3-methyl-1-butene and 2-methyl-1-butene), $LaCoO_3$ favored aldehydes (2-methylpropanal), and $LaNiO_3$ produced ketones such as 4-methylpentan-2-one. Raising temperature to 600°C shifted $LaMnO_3$/$LaCoO_3$ toward light carbonyls (acetaldehyde as dominant, with propanal and butanal), whereas $LaNiO_3$ enabled aromatization (toluene). Co-feeding methanol or ethanol promoted acetals (1,1-dimethoxyethane, 1,1-dimethoxypropane and 2-methyl-1,1-dimethoxypropane) and pentanoic acid; batch tests yielded ester-rich profiles (isobutyl octanoate; 2-methylpropyl acetate and 2-methylpropyl decanoate).

For ethanol conversion, ten Mg/Al-based catalysts were synthesized (M^{2+}/M^{3+} = 3/1 or 5/1), with partial substitution of Mg at different levels by Zn/Ni or Zn/Cu. At 400–500°C, Zn–Ni catalysts exhibited enhanced crotonaldehyde formation together with 1-butanol, ethyl butanoate, and butanal, consistent with coupled dehydrogenation–aldol sequences. Zn–Cu catalysts favored acetaldehyde and secondary products (2,3-dihydrofuran, acetone/2-pentanone, and methyl levulinate), evidencing fine tuning of the balance between redox and basic sites. Overall, perovskites and hydrotalcites provide, tunable platforms for integrated sugarcane-alcohol valorization into renewable chemicals.

These datasets show that catalyst composition (B-site transition metal or Zn-based substitution) and temperature steer the balance between dehydration, dehydrogenation, condensation, acetalization and aromatization. The resulting product slate spans C_2–C_5 carbonyls, C_4 unsaturated, acetals and esters—platform molecules for solvents and downstream upgrading.

Acknowledgements: FAPESP grants 2024/06046-7; 2024/10788-9 and 2025/01608-0.

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CCS - D1 - P06
Exploring electrically addressable catalysts for CO_2 valorization via dynamic catalysis

Marianna Angelo Tassioula[1], Gleb Ivanushkin[1], Giovanni Pampararo[1], Michiel Dusselier[1]
[1]KU Leuven, Belgium

Designing a high-performance catalyst requires fundamental knowledge of thermodynamics, reaction kinetics and structure-activity relationships. As described by the Sabatier principle, optimal catalyst activity only occurs at an intermediate adsorbate binding strength[1] (Figure 1). However, the recent emergence of dynamic catalysis offers a promising route to overcome these constraints[1]. The active site(s) in a dynamic catalyst undergo continuous changes during the reaction, creating the perfect environment for each individual elementary step. Via an applied stimulus, the adsorbate binding energies oscillate around the optimum at frequencies similar to those of the natural frequencies of the reaction, leading to catalytic rates that can exceed the Sabatier limit[1]. This results in enhanced catalyst performance, and may even provide a more selective pathway for existing processes that suffer from side product formation and harsh reaction conditions, such as CO_2 to methanol and methanation. In this work, a benchmark static catalyst system was first developed using commercial catalysts (Ni/SiO_2, $Cu/ZnO/Al_2O_3$) for the aforementioned reactions. Experimental testing is conducted in a continuous plug-flow reactor operating at industrially relevant temperatures and pressures. After optimizing reaction parameters, the feasibility of novel materials in classical thermocatalysis will first be quantified prior to implementing dynamic conditions. Innovative Cu- and Ni-based catalyst designs and reactor modifications (in collaboration with imec, UGent) will be investigated to evaluate their catalytic activity and performance alongside the ability to impart different stimuli. This non-traditional approach holds promise to drastically improve reaction kinetics and allowing for operation under milder reaction conditions.

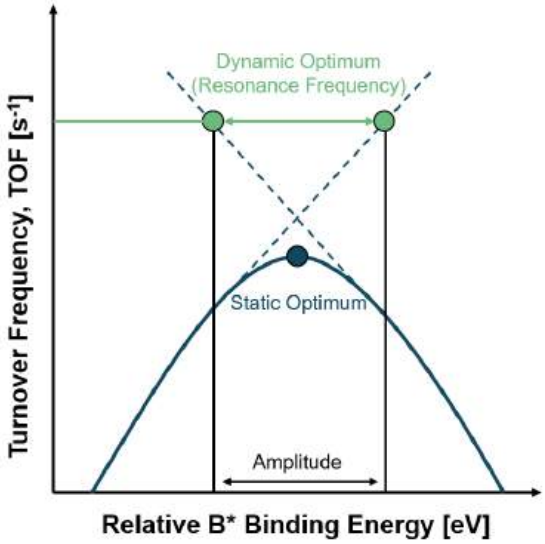

Fig. 1. A representation of dynamic catalysis. The optimum of a static catalyst highlighted at the apex of the Sabatier volcano plot, whereas a higher catalytic rate for a dynamic catalyst can be found at an maximum known as the resonance frequency. Adapted from [1].

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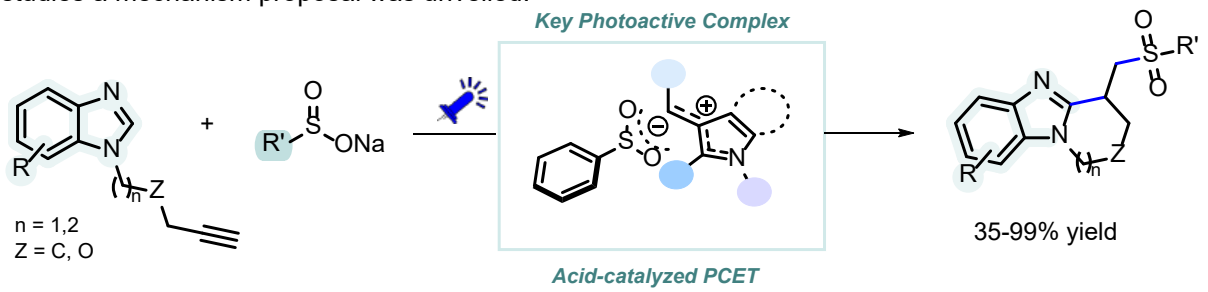
CCS - D1 - P07

Radical cascade sulfonylation/cyclization of benzenimidazole derivatives with sulfinates induced by visible light

Polyssena Renzi[1], Davide Cerrina[1], Giovanni Ghigo[1], Annamaria Deagostino[1]
[1]Dept. of Chemistry, University of Turin, Italy

Organosulfur moieties are key features in numerous natural products[1] and functional materials.[2] They are of particular interest to the pharmaceutical industry,[3] with over 150 sulfur-containing drugs currently available on the market.[4] Consequently, the development of milder and more environmentally friendly methodologies for the formation of C-S bonds has been the object of an intensive work for organic chemists. Photocatalysis has emerged as a central area of research, offering unique reactivity pathways that are challenging to achieve through traditional thermal transformations.

In recent years, our research group has focused its attention on the photoinduced generation of key sulfur-centered radicals, such as sulfonyl and thiyl radicals,[5-7] with the objective of utilizing them for the functionalization of unsaturated compounds. In this context, benzimidazole derivatives with appended alkyne functionality and sodium sulfinates have been employed as the starting materials in a radical cascade sulfonylation/cyclization mediated by bench-stable diarylmethylium tetrafluoroborate organo-photocatalysts under blue light irradiation.[7] More than 20 polycyclic sulfonyl-benzimidazoles, including azepines, are obtained in good to excellent yields, in mild and metal free conditions. Based on both experimental and computational studies a mechanism proposal was unveiled.



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CCS - D1 - P08
Progress and challenges in electrocatalytic oxidation of nitrogen compounds

Elisabeth T. Gallmeier[1], Dominik P. Halter[1]
[1]University of Antwerp, Faculty of Applied Engineering, Dept. of Biochemical and Chemical Engineering, Research Group Applied Electrochemistry & Catalysis (ELCAT), Belgium

Selective oxidation at the nitrogen of N-containing molecules, such as amines, imines, and di-nitrogen, is an important class of reactions with synthetic applications in pharmaceutical, food, and agricultural industries.[1,2] In contrast to traditional, thermal methods of N-oxidation, electrochemical synthesis offers a green, redox and energy efficient alternative that overcomes the need for high temperature and pressure conditions together with strong, toxic oxidants.[3] Besides the potential for improved selectivity, electrochemical methods of N-oxidation at the anode can be coupled to H_2 evolution, e-hydrogenation or other cathodic reductions for the synthesis of two value products in parallel.[4]
This work focuses on strategies for electrochemical N-oxidation using mixed-metal and doped metal oxide materials. Different electrolyte conditions and catalyst immobilization strategies are systematically evaluated, to optimize product selectivity, yield, and faradaic efficiency for different substrates. The fundamental insight will pave the way towards further performance improvement in the future through process engineering.

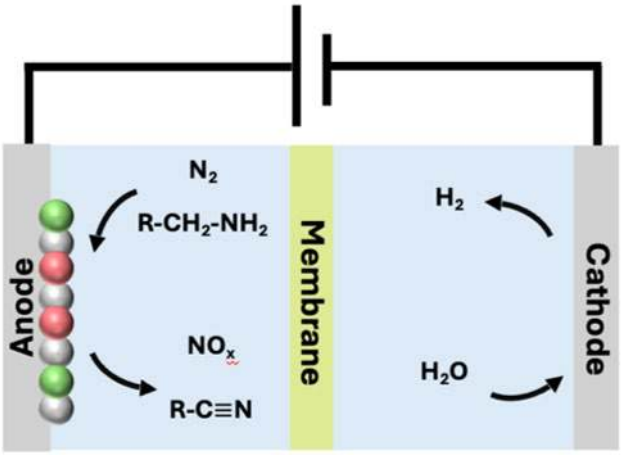

Fig.1. Electrocatalytic oxidation of nitrogen compounds on immobilized metal oxide materials

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CCS - D1 - P09

Role of calcination temperature of CuZnAl and CuZnGa catalysts for CO_2 hydrogenation to methanol

Gabriela Zanelli[1], Alessandra Lucredio[1], Alexandra Bouriakova[2], Willem De Meyer[2], Joris Thybaut[2], Elisabete Assaf[1]

[1]São Carlos Institute of Chemistry, University of São Paulo, Brazil; [2]Laboratory for Chemical Technology, Ghent University, Belgium

The catalytic hydrogenation of CO_2 to methanol is a promising pathway for carbon valorization, yet its large-scale implementation requires catalysts with high activity, stability, and structural tunability. CuZn based materials remain the benchmark, their performance strongly being governed by the physicochemical properties obtained during synthesis and thermal treatment.[1,2] In this work, we evaluate how calcination temperature determines the structure–performance relationships of CuZnAl and CuZnGa catalysts derived from hydrotalcite-like precursors.

Catalysts were prepared by coprecipitation and calcined at 330°C or 600°. Limiting the calcination temperature to 330°C favors the formation of smaller Cu^0 crystallites and preserves copper dispersion and exposed metal area. In contrast, calcination at 600°C promotes stronger metal–oxide interactions and possible copper sintering.[3,4] H_2 Temperature-Programmed Reduction reveals that Ga incorporation decreases the reduction temperature, suggesting the facilitated formation of active sites at both calcination temperatures.

Catalytic tests at 250°C, 30 bar, GHSV = 18,000 $mL.min^{-1}.g_{cat}^{-1}$ and H_2/CO_2 = 3 demonstrate that the CuZnGa catalyst calcined at 330°C exhibited significantly higher CO_2 conversion and methanol selectivity. The improved performance correlates with higher copper dispersion and greater accessibility of active sites. Although the CuZnAl sample exhibits inferior performance compared to the gallium-promoted catalyst at low calcination temperatures, both exhibit very similar results at higher calcination temperatures, indicating that promoter–support interactions and calcination temperature are key factors governing catalytic performance and that a high calcination temperature eliminates the impact of Al vs Ga. To further deepen the understanding of the catalyst structure and correlate it with catalytic performance, *in situ* X-ray diffraction analyses will be performed.

Overall, our work elucidates how promoter identity and thermal treatment control the physicochemical features of CuZn catalysts, enabling the rational design of next-generation materials for efficient CO_2-to-methanol conversion.

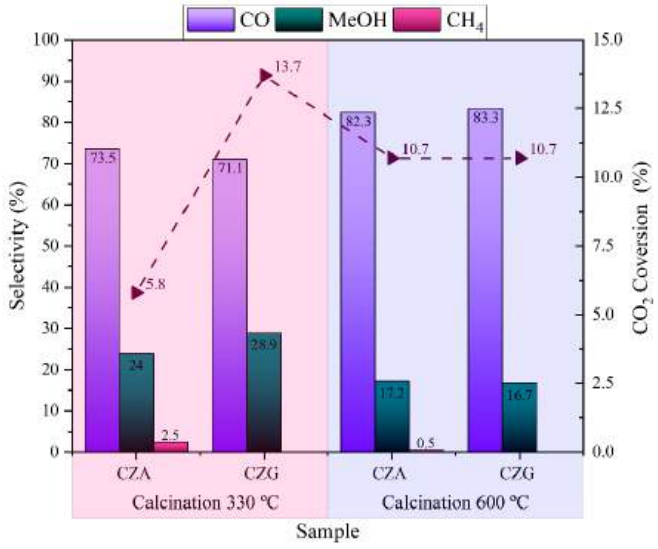

Fig. 1. Catalytic tests of the materials calcined at 330 ºC or 600 ºC

The authors acknowledge the financial support from FAPESP – São Paulo Research Foundation (Process Nº. 2024/00032-4 and Process Nº. 2025/09667-5) and from CNPq (Process Nº 300454/2025-2).

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CCS - D1 - P10
Catalytic conversion of a-pinene to high value products

Filippo Ravasio[1], Katharina Konieczny[1], Eszter Baráth[1]
[1]*Leibniz-Institut für Katalyse e.V. (LIKAT), Germany*

Turpentine oil, a byproduct of the paper industry, is a very attractive and highly available raw material. The main constituent of turpentine is a-pinene which can be used as a source of building blocks for the fine chemical industry (Figure 1). For example, *cis*-pinane is a valuable intermediate widely used in pharmaceutical synthesis and can be obtained through the selective hydrogenation of a-pinene.[1] The hydrogenation of the double bond can be carried out by catalytic transfer hydrogenation (CTH) using hydrogen donors or by direct hydrogenation using gaseous molecular hydrogen (H_2).[2] Another industrially relevant compound that can be produced from a-pinene is *p*-cymene, which is commonly used as an additive in fragrances.[3] Pt/C and Ru/C were tested with primary and secondary alcohols as hydrogen donors for the reduction of a-pinene to *cis*-pinane. While secondary alcohols exhibited complete conversion, primary alcohols were inactive. Overall, Ru/C showed higher selectivity towards the *cis* isomer compared to Pt/C under the same reaction conditions. The activation parameters of the reaction were determined and compared for the two systems. Isotope-labeling experiments were carried out to gain deeper mechanistic insights.
Regarding the conversion of a-pinene to *p*-cymene a series of noble and transition metals were tested. Rh-based catalysts showed the best performance in terms of conversion and selectivity. The influence of the support and of the pretreatment of the catalyst were examined, and different primary and secondary alcohols were studied as solvent. The overall plot of the reaction suggests a one pot reaction cascade involving an isomerization step followed by sequential dehydrogenation.

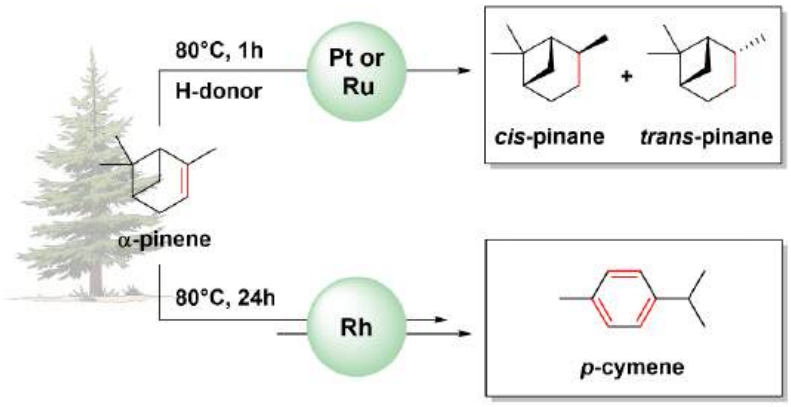

Fig. 1. Conversion of α-pinene to pinane and to *p*-cymene.

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CCS - D1 - P11

From batch to flow: Ammonia as a weak base for the synthesis and functionalization of Au, Pd, and Cu-NHC complexes

Riku Saito[1], Pierre Arnaut[1], Gianluca Carì[1], Leandros P. Zorba[1], Andreas Simoens[2], Celle Vandersteen[2], Christian Stevens[2], Catherine S.J. Cazin[1], Steven P. Nolan[1]

[1]Dept. of Chemistry, Center for Sustainable Chemistry, Ghent University, Belgium; [2]Dept. of Green Chemistry and Technology, SynBioC Research Group, Faculty of Bioscience Engineering, Ghent University, Belgium

The development of efficient and sustainable synthetic routes to *N*-heterocyclic carbene (NHC) complexes of late transition metals is crucial for advancing their applications in catalysis, materials science, and medicine. While traditional methods – such as the strong-base "free carbene" route or transmetalation from Ag/Cu-NHCs – often require inert conditions, toxic solvents, and generate significant waste, the milder "weak base route" has emerged as a more practical alternative.

Recently, aqueous[1-5] and gaseous[4] ammonia have been introduced as exceptionally economical, green, and effective weak bases for assembling a broad range of metal-NHC complexes. This approach enables reactions under ambient conditions, significantly reduces reaction times, simplifies workup via "phase-cut" aqueous extraction, and, in a representative case, dramatically lowers the environmental footprint (E-factor reduced from >500 to ~20).[2] Furthermore, the homogeneous nature of ammonia-based systems permits translation into continuous-flow setups, overcoming issues of previous state-of-the-art approaches – such as clogging and solubility limitations – and enabling higher reaction concentrations (up to 20 times more concentrated in a representative case than previous approaches), underscoring the higher efficiency and greener nature of this method.[4] This ammonia-mediated methodology has been successfully extended to the functionalization of metal-NHC complexes, such as the preparation of structurally diverse [Au(NHC)(Aryl)] complexes bearing polyaromatic aryl structures with potential photonic applications.[5]

By providing a cost-effective, operationally simple, and environmentally benign synthetic platform, the use of ammonia as a weak base significantly enhances the accessibility of well-defined metal-NHC complexes, accelerating their exploration across multiple disciplines.

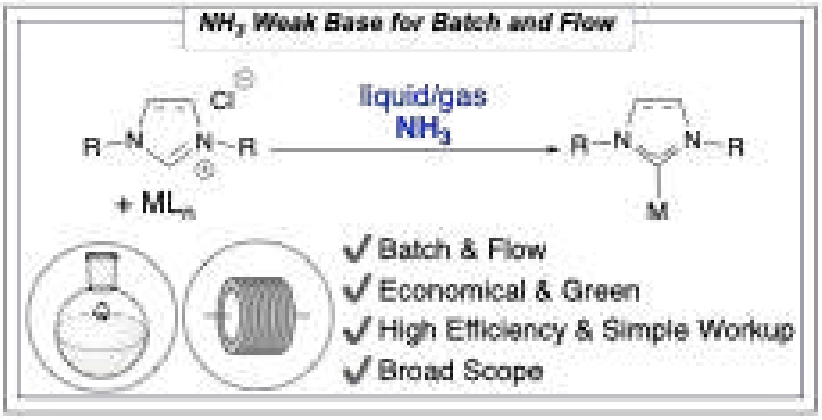

Fig. 1. Ammonia-mediated synthesis of metal-NHC complexes in batch and flow approaches.

[1]Saito, R. et. al. *Dalton Trans.* **2025**, *54* (1), 59–64.
[2]Saito, R. et .al. *Dalton Trans.* **2025**, *54* (30), 11720–11724.
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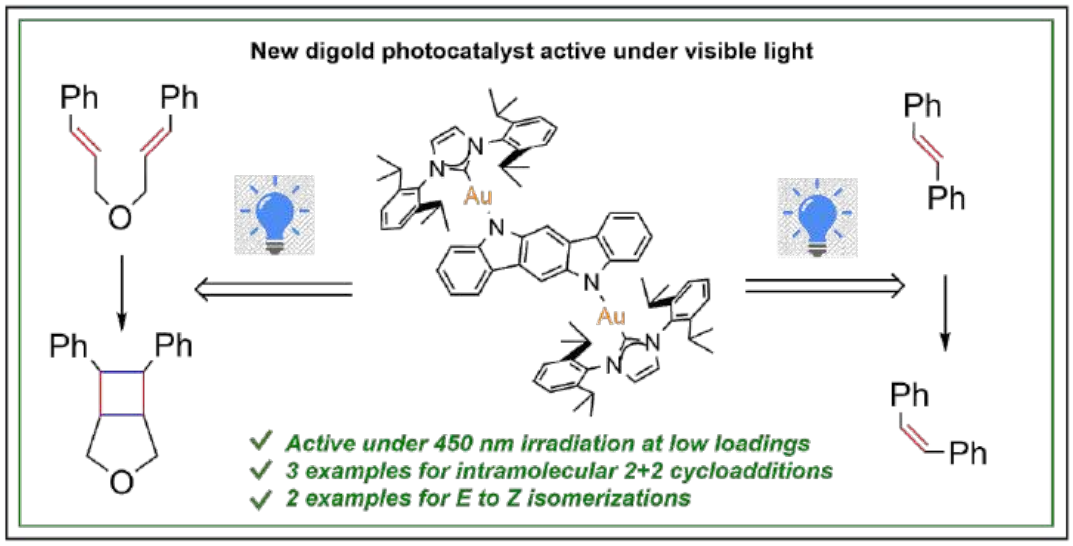
CCS - D1 - P12
Digold photosensitizer for visible light [2+2] cycloaddition and E/Z isomerization reactions

Tommaso Ruggiero[1], James Fortwengler[2], Kristof Van Hecke[1], Mark E. Thompson[2], Thomas S.A. Heugebaert[3], Steven P. Nolan[1]
[1]Dept. of Chemistry and Center for Sustainable Chemistry, Ghent University, Belgium; [2]Mork Family Dept. of Chemical Engineering and Materials Science, University of Southern California, USA; Dept. of Chemistry, University of Southern California, USA; [3]Dept. of Green Chemistry and Technology, Ghent University, Belgium

Energy transfer photocatalysis has emerged as a powerful platform for a wide variety of transformations, yet advances in this area are often limited by the visible-light absorption of catalysts and the very high cost of state-of-the-art iridium-based sensitizers. We report the synthesis, characterization, and photocatalytic use of a novel digold(I) complex, {[Au(IPr)]$_2$(DHIC)} (**PhotAu3**), designed to overcome these limitations by absorbing visible light in the blue region and proving catalytically effective under 450 nm LED irradiation.
PhotAu3 is obtained from addition of 2 equivalents of [Au(IPr)(OH)] to 5,11-dihydroindolo[3,2-*b*]carbazole (DHIC) in ethyl acetate. The complex exhibits a phosphorescence band with a peak at 562 nm, corresponding to a triplet energy (E_T) of 50.9 kcal/mol; its photoluminescence quantum yield (PLQY) is 3% and lifetime in THF is 39 µs. Crystal structure of PhotAu3 was confirmed through diffraction studies on single crystal and shows two spatial conformations of the molecule. The catalyst was deployed in two classes of EnT reactions: intramolecular [2 + 2] cycloadditions and E/Z isomerization. Under optimized conditions the cycloaddition of substrate cinnamyl ether reached quantitative conversion and high isolated yields (90 % in 30 minutes. 0.5 mol% of catalyst). For E/Z isomerization, Z/E ratios up to or 79/21 for stilbene were achieved within 1h using 0.5 mol% of catalyst. Conventional photosensitizers such as benzophenone or thioxanthone proved ineffective under the same conditions.
These results demonstrate that **PhotAu3** is the first gold-based complex to achieve efficient EnT photocatalysis under visible-light irradiation, offering a sustainable and cost-effective alternative to iridium-based sensitizers. Its low catalyst loading, short reaction times, and compatibility with blue-light LEDs highlight the potential of binuclear gold complexes for a variety of EnT-mediated synthetic applications.



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CCS - D1 - P13
CO_2 hydrogenation over MOF-derived carbon-modified copper catalysts

Angela Maria Kasza[1,2], Monica Dan[1], Mihaela Diana Lazar[1], Maria Mihet[1]
[1]National Institute for Research & Development of Isotopic and Molecular Technologies - INCDTIM, Romania;
[2]Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania

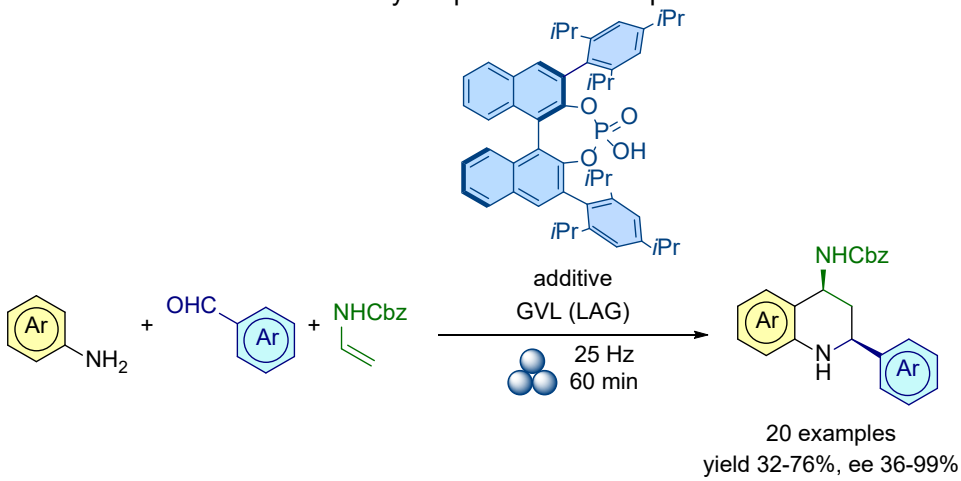
Growing scientific and technological interest in the valorization of carbon dioxide has intensified research on CO_2 hydrogenation to methanol (CO_2-MeOH). This reaction is attractive as a route for CO_2 mitigation, as a power-to-liquid energy storage option, and as an alternative pathway to conventional syngas-based methanol synthesis. Nevertheless, CO_2-MeOH remains highly challenging because of unfavorable thermodynamics, the chemical stability of CO_2, the occurrence of parallel reactions, and catalyst deactivation.
In this work, MOF-derived carbon was employed as a modifier for Cu/ZnO/Al_2O_3 (CZA) catalysts with a Cu:Zn:Al molar ratio of 6:3:1. The aim was to simultaneously increase the specific surface area, improve copper dispersion, and enhance water resistance of the catalysts, due to the hydrophobic character of the added carbon.The carbon material was obtained by inert thermal treatment of MIL-53(Al), synthesized via a cost-effective hydrothermal route, resulting in a channel-like porous carbon with a high surface area. Composite catalysts containing 3, 6, and 12 wt.% carbon were prepared by Na_2CO_3 co-precipitation at pH 7. Comprehensive characterization demonstrated uniform dispersion of the catalyst components, a slight increase in CuO particle size with increasing carbon content, enhanced surface area and pore volume, and a narrower pore size distribution. The addition of carbon significantly influenced reducibility as well as CO_2 and H_2 adsorption properties, indicating promising potential for improved catalytic performance in CO_2 hydrogenation to methanol.
Thermodynamic equilibrium was investigated using Gibbs reactor simulations in ChemCAD with the Soave–Redlich–Kwong equation of state to assess the influence of operating conditions. Catalytic activity tests were performed in a tubular fixed-bed reactor under plug-flow conditions. The effects of parameters on catalytic performance were investigated at reaction temperatures of 200-300 °C, pressures of 10-40 bar, GHSVs of 4800-14,500 h^{-1}, and H_2/CO_2 = 3-6 molar ratios.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV.

CCS - D1 - P14
Chiral Brønsted acid catalyzed mechanochemical stereoselective Povarov reaction

Péter Kisszékelyi[1], Terézia Doblejová[1], Erik Rakovský[2], Radovan Šebesta[1]
[1]Dept. of Organic Chemistry, Comenius University Bratislava, Slovakia; [2]Dept. of Inorganic Chemistry, Comenius University Bratislava, Slovakia

A mechanochemically-assisted Povarov reaction catalyzed by BINOL-derived Brønsted-acid organocatalyst enabled the stereoselective synthesis of various tetrahydroquinolines in good yields and high enantiomeric purities (Scheme 1). This organocatalytic transformation represents a new example for stereoselective mechanochemical transformations utilizing non-covalent interactions. The multicomponent reaction involves the condensation reaction of an aromatic amine and an aryl aldehyde, followed by the reaction of the corresponding imine with an electron rich alkene. The mechanochemical methodology was realized for both solid and liquid aromatic aldehydes. Various conventional and more sustainable solvents were tested for the liquid-assisted grinding (LAG), which showed that, other than the typically used solvents, more environmentally friendly variants (e.g., γ-valerolactone) can be suitable as well. Moreover, the mechanochemical process has significantly lower mass intensity than the solution-based procedures. The liquid-assisted grinding had a positive effect not only on chemical yields but also on the enantioselectivity of this transformation by allowing key interactions between the organocatalyst and the reagents. Furthermore, the screening of LAG solvents gave insight into the reaction mechanism. The isolation of an ethanol-adduct originating from a polar cationic intermediate and the significant effect of solvent polarity suggests a stepwise polar mechanism. DFT calculation provided further information on the stereoinduction of the reaction. In conclusion, this work shows that mechanochemistry is compatible with asymmetric organocatalytic transformations which rely on weak non-covalent interactions and can lead to more sustainable organocatalytic applications furnishing complex molecular structures in a relatively simple reaction setup.



Scheme 1. Chiral Brønsted acid catalyzed mechanochemical Povarov reaction.

This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00030 (PK).

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CCS - D1 - P15
Immobilized pincer ligand for cross-coupling reaction in flow

Fuline Musengo Otomboy[1], Christophe Vande Velde[1]
[1]*University of Antwerp, Belgium*

Nowadays, BASF uses up to 1% of the annual global Pd production for the synthesis of the agrochemical Xemium![1,2] In addition, the Suzuki-Miyaura reaction is the first chemical reaction in the industry[3]. All of this underscores the importance of sustainable management of palladium resources, as it is not possible to replace palladium in every application.
I am Fuline MUSENGO OTOMBOY, a PhD candidate at the University of Antwerp. Within the iPRACS research group, my project aims to immobilize a pincer ligand to use as a catalyst for the Suzuki-Miyaura reaction. The immobilization of the pincer is expected to affect the catalyst's rate; however, this is not a limitation for this project, as I aim to benefit from extended catalytic activity over a longer period, induced by the immobilization. How is this possible? Pincer ligands are known homogeneous catalysts, but homogeneous catalysts are limited by their reusability. To address this, the pincer will be covalently immobilized within a metal-organic framework (MOF). The MOF has been selected as the support material for its crystallinity and characterizability. With the MOF, we can characterize the catalyst throughout its life cycle. The functionalization rate of the MOF will be optimized to leverage its porosity for the catalytic reaction. In addition, the optimized functionalization rate is expected to allow the use of less Pd than in homogeneous conditions. The benchmark will compare the performance to its homogeneous counterpart. The Suzuki-Miyaura benchmark reaction will be the coupling of phenyl boronic acid with bromobenzene, using cesium carbonate as a base and Pd diacetate. This methodology is my solution for sustainable Pd resource management.

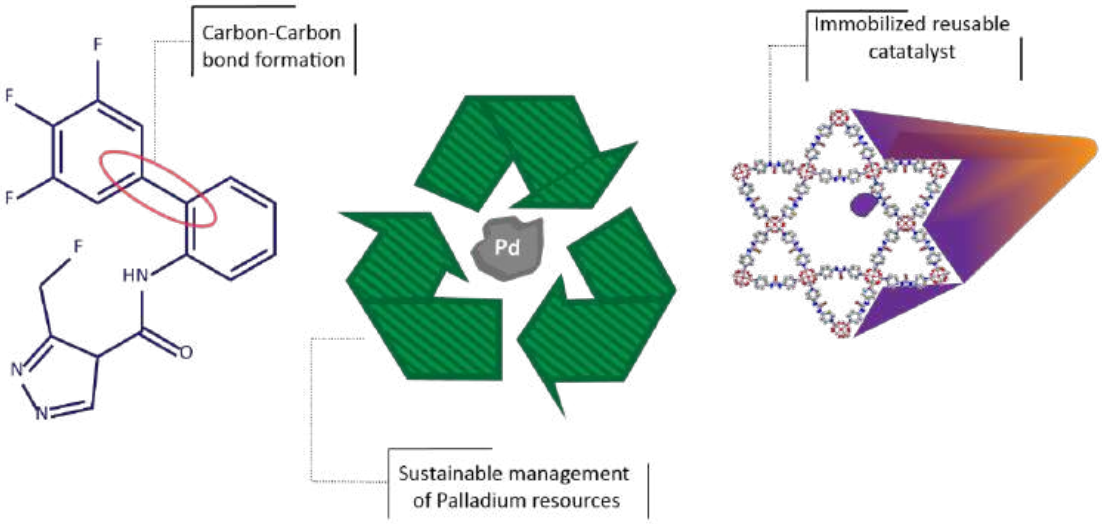

Fig. 3. visual abstract of Immobilized pincer ligand for cross-coupling reaction in flow

The FWO funds this project, grant number is 1SACG26N.

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[2]*Buchwald-Hartwig reaction: An overview - ScienceDirect*. https://www.sciencedirect.com/science/article/pii/S0022328X18301128?casa_token=U0OVKE2gR4UAAAAA:uBPEd1wB8oNeivQNgWA_Hs30bZfWwzJIxpXOHXREdnofOAvkGp7LQrPoPs0jjjRgtsl7ph9QWg (accessed 2025-01-09).
[3]Farhang, M.; Akbarzadeh, A. R.; Rabbani, M.; Ghadiri, A. M. A Retrospective-Prospective Review of Suzuki–Miyaura Reaction: From Cross-Coupling Reaction to Pharmaceutical Industry Applications. *Polyhedron* **2022**, *227*, 116124. https://doi.org/10.1016/j.poly.2022.116124.

CCS - D1 - P16

Potential of tubular continuous flow photoreactors for plasmonic photocatalytic reverse water gas shift process

Sophie Mansvelders[1], Roberto Habets[1], Jonathan van den Ham[1], Jordi Volders[1], Silvia Zanoni[1], Nicole Meulendijks[1], Pascal Buskens[1,2]

[1]The Netherlands Organization for Applied Scientific Research (TNO), The Netherlands; [2]Hasselt University, Institute for Materials Research (imo-imomec), DESINe Group, Belgium

CO_2 capture and utilization (CCU) technologies are expected to play an important role in reducing emissions and enabling sustainable chemical production.[1] A CCU technology is the reverse water gas shift (rWGS) reaction, in which CO_2 and green H_2 are converted into CO and H_2O. The resulting CO, together with H_2, serves as a feedstock for methanol synthesis and long-chain hydrocarbons via the Fischer Tropsch process. Therefore, the rWGS reaction can serve as first step for the production of synthetic fuels and chemicals from CO_2.[2]

The rWGS reaction is endothermic and equilibrium limited. In thermocatalysis, temperatures above 800 °C are required to achieve CO selectivity above 80% while suppressing methanation. Plasmonic catalysis provides an alternative by using metallic nanoparticles to harvest energy of (sun)light and drive the reaction.[1] However, photocatalytic studies often rely on batch reactors, which limit the CO production rate per m^2 of illuminated catalyst bed and therefore hinder translation towards industrial application.[1]

To address these challenges, we developed a tubular continuous flow photoreactor designed to increase the effective optical path length without compromising throughput, thereby maximizing the CO production rate per m^2 of illuminated catalyst bed, while also identifying the limitations of the setup. Using a TiO_2-supported Au nanocatalyst in a packed-bed configuration, the reactor achieved full CO selectivity under low pressure, moderate temperatures and mildly concentrated artificial sunlight (10 bar, 200 °C, 6.0 $kW \cdot m^{-2}$ = 6.0 suns), demonstrating the potential of plasmonic photocatalysis for CCU. However, CO production rates remained limited, likely due to the limited solar intensity.

These findings highlight the challenges and potential of the current tubular continuous flow photoreactor in advancing photocatalytic rWGS towards practical applications in solar driven synthetic fuel production.

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CCS - D1 - P17
Tuning the porosity and structure of the oxidic supports to enhance the catalytic efficiency

Monica Dan[1], Oana Grad[1], Angela Kasza[1], Maria Mihet[1], Diana Lazar[1]
[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Romania

In this modern and industrial society, it is vital to find solutions for converting CO_2 into a sustainable resource, thus trying to control climate change and build a circular carbon economy [1]. This process relies on advanced catalyst classes such as heterogeneous, single-atom, advanced metallic frameworks that are specifically designed to improve the process efficiency and selectivity.
Due to their high surface areas and thermal stability, the alumina and silica oxides are the primary supports used for various catalytic materials active in CO_2 conversion processes.
Although both alumina and silica supported metal catalysts are valued for their improved properties, like strong metal-support interactions, acid-base sites, CO_2 adsorption, and high dispersion, research is still needed to improve the selectivity and long-term stability of these catalysts for producing fuels like methane and methanol [2,3]. By modifying the porosity and structure of the catalytic materials, we aim to enhance reaction kinetics to transform the CO_2 into high-value fuels and chemicals.
In our study, we investigate the possibility of adding La and Ce to the silica support with multimodal porosity and designing the alumina support porous structure in order to enhance the CO_2 transformation. The newly obtained doped metallic-silica support catalysts exhibit an improved metal dispersion and a higher catalyst stability, leading to higher conversion rates and superior selectivity. The synthesized bimodal alumina structure presents a dual pore architecture featuring macropores and mesopores. We observe that the tested bimodal catalysts exhibit improved mass transport and resistance to coke formation, reflected in higher conversion rates and a superior thermal stability for the production of methane and synthesis gas.

Acknowledgements: The funding for this research was provided by: PN-IV-P6-6.1-CoEx-2024-0053
Chemo-catalytic paradigms in multiphase waste valorization – Center of Excellence for Circular Chemistry and Economy

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CCS - D1 - P19
Influence of the MOF-derived carbon-type promoters on CO_2 hydrogenation to methanol

Angela M. Kasza[1,2], Monica Dan[1], Mihaela D. Lazar[1], Maria Mihet[1]
[1]National Institute for R&D of Isotopic and Molecular Technologies – INCDTIM, Romania; [2]Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania

Due to the growing interest in CO_2 valorization pathways, CO_2 hydrogenation to methanol (CO_2–MeOH) has received significant attention recently, especially as an alternative for chemical energy storage (the power-to-liquid concept – P2L). The most important challenges of CO_2–MeOH are the competitive reverse water gas shift reaction (RWGS), which leads to low methanol selectivity at higher CO_2 conversion, as well as catalyst deactivation due to water formation. In this regard, one strategy in designing selective and stable catalysts for CO_2–MeOH is the use of hydrophobic high surface area carbon materials as promoters, thus favoring the dispersion of catalytic components and providing enhanced water resistance. In this work, two types of MOF-derived carbon structures were used to promote the classical Cu-ZnO-Al_2O_3 (CZA) catalyst. These two ordered mesoporous carbon structures were obtained by thermal treatment of MIL-53(Al), a flexible, microporous Al-based metal-organic framework, synthesized via a cost-effective hydrothermal route established in our group[1]. As a consequence of the Al presence in the initial MOF, an alumina-doped carbon, C_{as}, is obtained by thermal treatment in Ar flow, at 600°C for 5 h, while the alumina-free carbon structure (*C*) was obtained by 10% HCl treatment of C_{as} at 80°C for 5 h. The promoted materials with carbon loadings of 6 wt.% were prepared by precipitation with Na_2CO_3 or $NaHCO_3$ of metal salt solutions containing Cu:Zn:Al = 6:3:1 in the case of *C*-CZA, or solutions containing only Cu:Zn = 6:3 for C_{as}-CZA, since C_{as} is an alumina-doped structure. Comprehensive characterization of *C*-CZA and C_{as}-CZA materials by XRD, BET, SEM/TEM/EDX, TPR, H_2/CO_2-TPD, FT-IR, DRIFTS, and N_2O titration revealed uniform dispersion of the components, enhanced surface area due to carbon modification, better reducibility, and different interactions with H_2 and CO_2, with subsequent differences in catalytic performance in the CO_2–MeOH process.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CNCS - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV.

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CCS - D1 - P20
Synthesis, characterization, and aggregation properties of cobalt-phthalocyanine

Birhan Tutal[1], Çağla Akkol[1], Ece Tuğba Saka[1], Serhat Avnikli[1]
[1]Karadeniz Technical University, Faculty of Sciences, Dept. of Chemistry, Turkey

Phthalocyanines (Pcs) are macrocyclic molecules that exhibit high aromatic character due to their conjugated 18π-electron systems. These structures are 16-membered (8 carbons, 8 nitrogens) planar macrocycles composed of four iminoisoindoline/benzo subunits. They possess high thermal and chemical stability owing to their extensively conjugated π-electron systems. Due to their planar structures and π-electron systems, phthalocyanines tend to undergo aggregation in solution. Aggregation occurs through the face-to-face (H-type) or edge-to-edge (J-type) stacking of molecules, which leads to shifts in the ultraviolet-visible (UV-vis) spectra. The formation of aggregation leads to a decrease in the intensity of the Q band, splitting, or shifts in wavelength (H-type blue shift, J-type red shift) in UV-Vis spectra, while also presenting structural characterization challenges such as the broadening of signals in NMR spectra.
The inherently low solubility of phthalocyanines can be enhanced by substituting the periphery of the macrocycle with bulky groups or long-chain substituents. To overcome these adverse effects and enhance both solubility and efficiency, the primary focus of research is to prevent aggregation by incorporating bulky or long-chain substituents onto the phthalocyanine macrocycle. In this context, 4-(cis-2,6-dimethylmorpholino)phthalonitrile was synthesized by the reaction of cis-2,6-dimethylmorpholine with 4-nitrophthalonitrile. Subsequently, the resulting phthalonitrile derivative was utilized as a precursor to obtain the corresponding cobalt phthalocyanine complex. The aggregation properties of the phthalocyanine were investigated using UV-Vis spectroscopy in various solvents and at different concentrations to examine the spectral changes, particularly in the Q and B bands.

Keywords: Phthalocyanine, aggregation.

This work was supported by Karadeniz Technical University, Trabzon, Turkey, under Scientific Research Projects Coordination Unit (Project Number:17061).

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CCS - D1 - P21

Unravelling surface mechanism in isopropanol dehydration to propylene: The impact of acid-base sites strength and nature

Tristan Cabanis[1], Aline Auroux[1], Jean-Luc Dubois[2], Nicolas Sbirrazzuoli[3], Georgeta Postole[1]
[1]Université Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, France; [2]Trinseo Netherlands B.V., The Netherlands; [3]Institut de Chimie de Nice (ICN) – UMR CNRS 7272, Université Côte d'Azur (UCA), France

This work compares the behaviour of three bulk oxides to elucidate the dependence of the surface mechanisms involved in the dehydration of isopropanol (IPA) to propylene (PEN) on the acid-base characteristics of the catalyst. Niobium oxide, magnesium oxide and alumina were selected for this study due to their distinct acid-base properties, namely solely acidic, solely basic and amphoteric, respectively. This high contrast makes it possible to isolate the influence of site nature and strength on each step of the catalytic process, i.e. adsorption, reaction and desorption. These 3 steps of the reaction were evidenced using a reactor inside a microcalorimeter linked to gas chromatography.[1]
Key findings:

- Acid sites are essential to coordinative adsorbed IPA and to trigger a surface reaction under catalytic conditions.
- Basic sites alone only exhibit a weak physical adsorption under inert flow. However, they may facilitate alcohol dissociation and enhance alkoxide formation on nearby acidic sites.
- Apparent activation energies reveal dual elimination pathways on alumina (E2 and $E1_{cb}$), while niobium oxide exclusively follows an E1 mechanism. These results highlight the important role of site nature and distribution in the surface mechanism.

Mixed data, from static and dynamic measurements, were used to accurately correlate surface properties with reaction mechanisms. The complementary nature of infrared and microcalorimetric methods combined with in situ measurements of adsorption and reaction/desorption heats (Figure 1.a) added to the kinetic computation of calorimetric signals (Figure 1.b) enables to improve the comprehension of fundamental surface mechanisms of acid-base heterogeneous reactions.

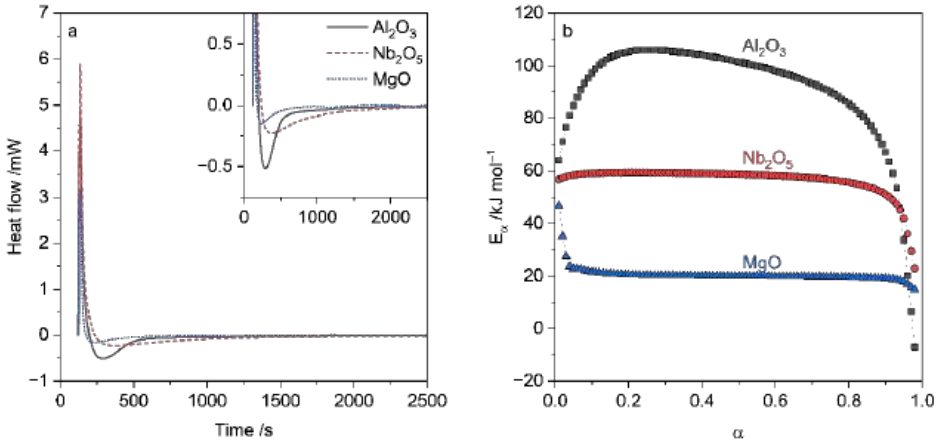

Fig. 4. Calorimetric signals recorded after IPA pulses (a) and related dependences of the effective activation energy versus the extent of conversion (b) obtained on alumina (solid, black), niobium oxide (dash, red) and magnesium oxide (dot, blue) at 175 °C.

This work is part of PYROCO2 project that has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 101037009.

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CCS - D1 - P22

Nanostructured molybdenum sulphide encapsulated in carbon spheres as stable and efficient electrocatalysts for the hydrogen evolution reaction

Rebeca Molina-Bueno[1], David Ruíz-Almóguera[1], José A.Mata[1], Iván Sorribes[1]
[1]Institute of Advanced Materials (INAM), Universitat Jaume I, Spain

Noble metal-free electrocatalysts are being developed for the hydrogen evolution reaction (HER) to enable the sustainable production of hydrogen from renewable energy sources. Among transition metal sulphides, molybdenum disulphide (MoS_2) offers an attractive combination of low cost and catalytic activity. However, its stability under electrochemical conditions is somewhat limited.[1,2]

This study presents a synthetic strategy involving the encapsulation of nanostructured molybdenum sulphides, prepared from molecular clusters,[1-4] within glucose-derived carbon spheres to improve the catalyst's stability. The electrocatalytic behaviour of the resulting materials was systematically evaluated by varying the content of molybdenum sulphide and optimising the preparation parameters.

Electrochemical stability was evaluated by performing 1000 consecutive potential sweeps and comparing the potential required to reach a current density of −10 $mA \cdot cm^{-2}$ in the first and last sweeps. Materials with encapsulated nanomaterials exhibited minimal variation in this potential, whereas significantly greater change was observed in non-encapsulated systems, indicating faster deactivation. These results demonstrate that carbon encapsulation slows down catalyst degradation and significantly improves its electrochemical stability, highlighting the potential of cluster-derived molybdenum sulphides as efficient and stable HER electrocatalysts.

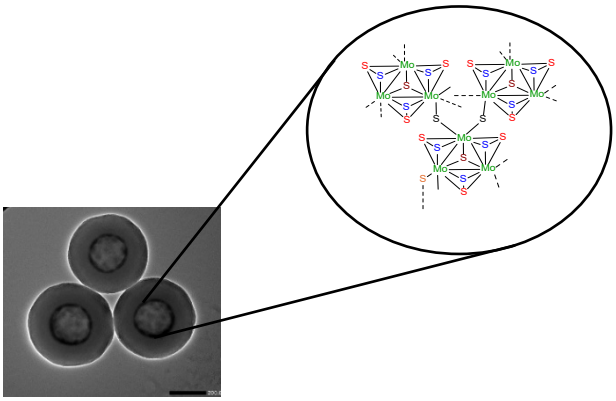

Fig. 1. Nanostructured molybdenum sulphide encapsulated into carbon spheres

Acknowlegements: The Grant ESGENT/016/2024 funded by the Gen-T Plan of the Generalitat Valenciana, as well as the grant PID2022-143164OA-I00 funded by MICIU/AEI/10.13039/501100011033 and by "ERDF/EU" are gratefully acknowledged.

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CCS - D1 - P23

Engineering nanostructured molybdenum sulphides for effective photocatalytic H_2 generation

Lidón Arroyas[1], María Calas[1], Javier E. Durantini[1], Sixto Giménez[1], Jose A. Mata[1], Iván Sorribes[1]
[1]*Institute of Advanced Materials (INAM), Universitat Jaume I, Spain*

Due to growing concern about the environmental impact of fossil fuels, there is increasing interest in the development of environmentally friendly energy sources. Hydrogen occupies a prominent position as an efficient and clean energy carrier, and its use as a sustainable alternative to fossil fuels can help tackle both environmental pollution and energy shortages. While conventional hydrogen production methods are energy-intensive, photocatalysis offers a simpler and more sustainable approach.

Molybdenum disulphide (MoS_2)-based nanomaterials are promising noble-metal-free co-catalysts for photocatalytic applications. Their catalytically active sites are located at the edges of the material; however, their performance is limited by the largely inert basal planes. Herein, we report an innovative bottom-up synthetic strategy in which molecular clusters are used as precursors to engineer sulphur-deficient and sulphur-enriched MoS_2-type nanomaterials. The resulting $\{Mo_3S_{4\text{-}7}\}_n$ nanomaterials feature coordinatively unsaturated atoms distributed throughout their structure, providing a high density of accessible active sites.[1-4] Consequently, when these nanomaterials are prepared in the presence of titanium dioxide (TiO_2), a widely used UV-responsive photocatalyst, result in efficient photocatalysts towards the hydrogen evolution reaction (HER) from water. Furthermore, $\{Mo_3S_7\}_n$ has been shown to function as a universal co-catalyst, exhibiting effective activity when combined with other inorganic semiconductors (g-C_3N_4, CdS, and MXene) as well as organic photosensitizers (erythrosine B sodium salt and eosin Y).

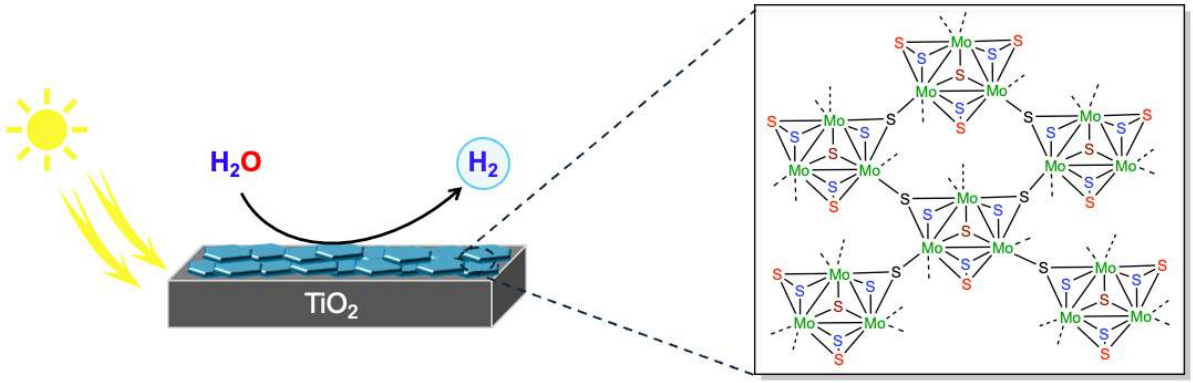

Fig.1. Photocatalytic HER catalysed by $\{Mo_3S_{4\text{-}7}\}_n/TiO_2$ nanocomposites

Acknowlegements: This work has been supported by the Grant PID2022-143164OA-I00 funded by MICIU/AEI/10.13039/501100011033 and by "ERDF/EU", as well as the Grant CNS2022-136183 funded by MICIU/AEI/10.13039/501100011033 and by "European Union NextGenerationEU/PRTR". The Grant ESGENT/016/2024 funded by the Gen-T Plan of the Generalitat Valenciana is gratefully acknowledged as well.

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CCS - D1 - P24
Formic acid dehydrogenation catalysed by nanostructured molybdenum sulphides

Markel Letona[1], Jose A. Mata[1], Iván Sorríbes[1]
[1]Institute of Advanced Materials (INAM), Universitat Jaume I, Spain

In recent years, the transition towards more sustainable and greener chemistry has gained increased interest, especially regarding the efficient and safe use of hydrogen as an energy vector. Within this context, formic acid has emerged as an attractive liquid organic hydrogen carrier due to its low toxicity, easy handling and its high volumetric hydrogen content. For this purpose, in this work, we report a catalytic methodology for the dehydrogenation of formic acid under moderate reaction conditions using ammonium formate as the reducing agent.
The keystone for the successful reaction is centred in the use of a sulphur-deficient molybdenum disulphide (MoS_2)-type catalyst, named $\{Mo_3S_4\}_n$, which is derived from molecular cluster precursors[1-4]. This nanomaterial has a large number of structural defects, both at the border positions and along the typically inert basal planes, which significantly increases its catalytic activity. This unique structure has made it possible to achieve efficient and reproducible conversion of formic acid into hydrogen and carbon dioxide. In addition, it has been demonstrated that the catalyst exhibits good recyclability over several consecutive runs, without a decrease in hydrogen production.

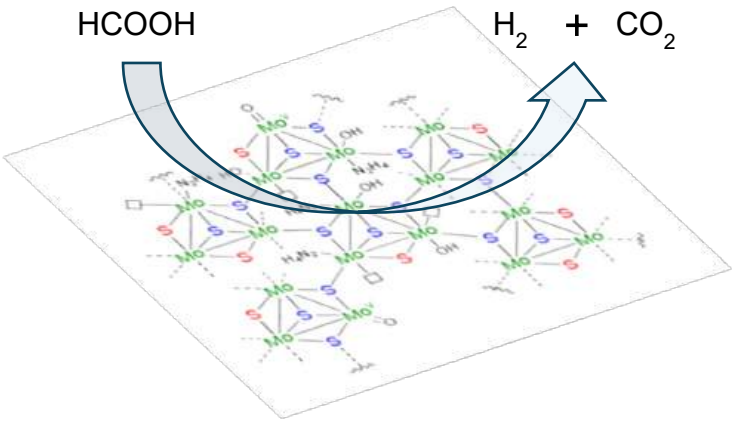

Fig. 5. $\{Mo_3S_4\}_n$-catalysed dehydrogenation of formic acid

Acknowledgements: The Grant CNS2022-136183 funded by MICIU/AEI/10.13039/501100011033 and by "European Union NextGenerationEU/PRTR", as well as the Grant ESGENT/016/2024 funded by the Gen-T Plan of the Generalitat Valenciana are gratefully acknowledged.

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CCS - D1 - P25
Ni_xCo_y for RWGS: A composition study

Jaime Cervera[1,2], Katerina Soulantika[1*], Juan Manuel Asensio-Revert [2], Malika Boualleg[2], Bruno Chaudret[1*]
[1]Laboratoire de Physique et Chimie des Nano-objets (LPCNO), France; [2]Ifp Energies Nouvelles, France

The concern over rising CO_2 levels on the atmosphere has been shaping world politics and science, promoting a circular carbon economy, to reduce our overall carbon footprint. The intrinsic thermodynamic stability of CO_2 has historically rendered it as a waste product from the combustion of organic matter and more specifically fossil fuels.[1,2] However, advances in science technologies (power-to-gas, dry reforming), have given CO_2 a new value as it is becoming an important C1-feedstock precursor in the industry. The Reverse Water Gas Shift (RWGS) enables the conversion of CO_2 into CO, which has an important role in industry, for instance, in the Fischer-Tropsch reaction.[3,4] Traditionally, the RWGS has been catalysed by noble metal-based catalysts, though their low abundance and high price limit their industrial application.[5] Non-noble metal-based catalysts, on the other hand, are usually less active and/or selective than their noble metal counterparts. Nevertheless, the combination of 2 different non-noble metals into a bimetallic catalyst might result in a synergistic effect, boosting activity and enhancing selectivity.[6] The RWGS, a complex reaction that is affected by the composition the catalyst active phase, can be used to probe the effects of bimetallicity. In this work, we present the synthesis via the organometallic method and the characterization through several techniques (XRD, XPS, HRTEM-EDX and TPD) of nickel-cobalt bimetallic catalysts (Ni_xCo_y/SiRAlOx and Ni_xCo_y/TiO_2), and their performance in the RWGS. Our results show that the Ni:Co ratio results in changes in the electronic ad structural properties that lead to different selectivity and activity.

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CCS - D1 - P26

Alkali-promoted iron-based catalysts for efficient and selective CO_2 hydrogenation to light olefin: A combined mechanistic and DFT insights

Babar Ali[1], Saheed A Ganiyu[1,2]

[1]*Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia;* [2]*Dept. of Chemistry, King Fahd University of Petroleum & Minerals, Saudi Arabia*

The hydrogenation of CO_2 to light olefins over alkali-promoted iron catalysts offers a sustainable pathway for CO_2 utilization and production of valuable chemicals. This study investigates the effect of alkali (Na, K, Cs) promotion on Fe-based catalysts for CO_2 hydrogenation to light olefins. Characterization techniques revealed that alkali promoters enhanced CO_2 adsorption, activation, and catalyst basicity, while weakening H_2 binding and facilitating desorption, shifting selectivity toward light olefins (C_2-$C_4^=$). The K-promoted catalyst achieved 38.3% olefin selectivity at 44.7% CO_2 conversion, attributed to stabilization of χ-Fe_5C_2 and suppression of alkene hydrogenation via moderate electron donation. In contrast, Na delayed Fe reduction and promoted heavier hydrocarbons, while Cs showed weak CO_2 uptake. XPS analysis revealed that K promotion enhances iron carburization, stabilizing the active χ-Fe_5C_2 phase and increasing the C-Fe fraction, which favors light olefin formation. In contrast, Na promotion leads to more oxidized Fe^{2+}/Fe^{3+} species and oxygenated carbon deposition, promoting heavier hydrocarbon growth. The higher surface carbide content and lower oxidation state in KFe catalysts correlate directly with higher olefin selectivity. In situ DRIFT revealed that CO_2 hydrogenation proceeds via a combined associative-dissociative pathway involving formate, carbonate (CO-C*), and CO intermediates, which transform into Fe-carbide species to drive C-C coupling. DFT simulations determined that alkali doping significantly alters the electronic structure and CO_2 adsorption behavior of Fe_2O_3 surfaces, with the (110) facet being the most active. K doping provided optimal adsorption energy (-0.80 eV) and balanced charge transfer, enhancing CO_2 activation and light olefin selectivity. In contrast, Na led to over-strong adsorption, resulting in heavier hydrocarbons, while Cs showed weak CO_2 binding and low activity.
Keywords: CO_2 hydrogenation, Iron Catalyst, olefins, alkali promoters, Iron carbide

Acknowledgements: The authors acknowledge the support and resources provided by the Interdisciplinary Research Center for Refining & Advanced Chemicals and the Dept. of Chemistry at King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia, under project No. INRC 2522

CCS - D2 - P01
Photocatalytic performance of phthalocyanine-based catalysts in the degradation of chlorophenols

Cagla Akkol[1], Ece Tugba Saka[1]
[1]Karadeniz Technical University, Türkiye

Photocatalysis is one of the promising techniques used in the degradation reactions of organic pollutants and is gaining increasing attention. Nowadays, using economical and environmentally friendly solvents, especially water, is of great importance in terms of green chemistry [1]. Chlorophenols are organic pollutants with high toxicity and environmental persistence, formed by the attachment of one or more chlorine atoms to a phenol ring. Chlorophenols, which enter aquatic environments through industrial wastewater, can remain in the environment for a long time due to their resistance to natural degradation.
In recent years, MPCs have attracted significant attention in catalysis due to the high catalytic activity of MPc that can be associated with central metal ions [2]. Cobalt and copper phthalocyanine (CoPc and CuPc), as transition metal complex catalysts with M-N4 active center, are among the most promising catalysts for this task due to their high activity and selectivity in oxidation processes[3]. Graphitic carbon nitride (g-C_3N_4) is a metal-free, chemically stable semiconductor with a suitable band gap that enables visible-light-driven photocatalysis. Owing to its low cost and facile synthesis, it has attracted significant attention for applications such as water splitting, CO_2 reduction, and environmental using photocatalytic processes [4]. In the study The photocatalytic performances of metallophthalocyanines/graphitic carbon nitride composites will be systematically investigated for the degradation of chlorinated phenolic pollutants, namely 2-chlorophenol, 2,3-dichlorophenol, and 2,3,6-trichlorophenol, under visible-light irradiation.
Keywords: Photocatalysis, phthalocyanine, chlorophenols

This study was supported by The Research Fund of Karadeniz Technical University (Project no: 16562)

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CCS - D2 - P02

Triple-active-site synergy in cu-doped ZIF-8 derived carbons enabling highly efficient hydrogen production

Hui Xu[1]
[1]FuDan University, China

A triple-active-site synergistic catalyst was designed for highly efficient hydrogen production via plasma-assisted seawater splitting. A series of Cu-doped ZIF-8-derived carbon catalysts were synthesized, among which Cu/Z-700 delivered the highest activity, producing 1.33 ml/min of H_2 at a short residence time of 3 s. Its exceptional performance originates from the synergistic interplay among three complementary active sites: Cu-cluster, Cu-NC and pyridinic nitrogen (Py-N). Bader charge analysis confirmed a reversible $Cu^0 \leftrightarrow Cu^+/Cu^{2+}$ redox cycle under DBD discharge, enabling dynamic charge exchange and radical formation. DFT calculations further revealed that Cu-cluster sites exhibit the strongest Cu–OH binding and the lowest reaction barriers, while Cu-NC sites offer moderate binding favorable for intermediate conversion and product release. Meanwhile, Py-N sites assist in water adsorption and interfacial charge redistribution. These results highlight the cooperative functions of the three active sites and provide fundamental guidelines for designing advanced plasma-assisted hydrogen production catalysts.

This work was supported by Shanghai Municipal Bureau of Ecology and Environment (Shanghai Eco-Environment Bureau SciTech[2025])

CCS - D2 - P03

Investigation of corrosion and antibacterial properties of triazole groups submitted CO(II) and MN(III) phthalocyanines coated C1018 alloy surfaces

Ismail Uzunel[1], Ece Tugba Saka[1], Olcay Bekircan[1], Salih Durdu[2,3], Ömer Kesmez[4]
[1]Karadeniz Technical University, Dept. of Chemistry, Turkey; [2]Giresun University, Dept. of Industrial Engineering, Turkey; [3]Giresun University, Dept. of Genetics and Bioengineering, Turkey; [4]Akdeniz University, Dept. of Chemistry, Turkey

Phthalocyanines which are heterocyclic compounds, have taken interest in applying as functional materials such as chemical sensors, liquid crystals, photovoltaic cells, optical data storage, organic semiconductors, catalysts, organic light emitting diodes (OLEDs), anticancer agents, electrochemistry, photodynamic therapy, due to their unique structural properties [1]. C1018 alloy (AISI 1018 low-carbon steel) is widely used in various industrial applications due to its good formability, weldability, and adequate mechanical properties. It is commonly employed in the manufacturing of shafts, bolts, gears, machine components, and structural parts, particularly in the automotive, manufacturing, and machinery industries, where cost-effectiveness and ease of machining are essential. However, owing to its low alloying element content, C1018 steel exhibits limited inherent resistance to corrosion. Preventing corrosion is therefore of critical importance to maintain mechanical integrity, extend service life, and reduce maintenance and replacement costs. Consequently, the application of corrosion protection strategies such as surface coatings, surface modification techniques, corrosion inhibitors, and controlled environmental conditions is essential for the reliable and long-term use of C1018 steel in engineering applications. [2].
In this study, triazole-substituted Co(II) and Mn(III) phthalocyanine compounds were first synthesized and systematically characterized. Subsequently, these compounds were electrochemically deposited onto C1018 steel surfaces, and the coated surfaces were characterized using FTIR, XRD, and SEM analyses. In addition, contact angle measurements were performed to evaluate the surface wettability properties. Activity tests against E. coli and S. aureus bacteria were then performed on the coated surfaces under both dark and daylight conditions.

This study was supported by The Scientific and Technological Research Council of Turkey (TUBITAK 125Z115).

Keywords: Phthalocyanine, corrosion, coating

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CCS - D2 - P04

Synthesis, characterization, and chemometric optimization of a DLLME method for Cu^{2+} determination using metal free phthalocyanine

İsmail Uzunel[1], Halil İbrahim Özen[1], Anıl Arda Günültas[1], Yasemin Caglar[2], Ece Tugba SAKA[1]
[1]Karadeniz Technical University, Dept. of Chemistry, Turkey; [2]Giresun University, Dept. of Genetics and Bioengineering, Turkey

Phthalocyanines have been widely employed as effective chemosensors for metal ion determination due to their extended π-conjugated structures and suitability for peripheral functionalization. In particular, phthalocyanine derivatives bearing donor atoms at their peripheral positions enable strong metal–ligand interactions, allowing for sensitive and selective analytical applications [1]. In addition, dispersive liquid–liquid microextraction (DLLME) has emerged as an efficient and environmentally friendly sample preparation technique owing to its low solvent consumption, high enrichment factors, and short extraction times [2, 3].
In this study, a novel metal free phthalocyanine peripherally functionalized with oxygen-containing ether groups was synthesized and fully characterized for the first time. The potential of the newly synthesized compound as a chemosensor for Cu^{2+} determination was investigated, and its applicability in a DLLME-based analytical system was evaluated for the first time. Phthalocyanines are well known for their strong π-conjugated structures, remarkable optical properties, and effective interactions with metal ions, making them attractive candidates for analytical sensing applications [4]. In this context, the synthesized Pc compound, possessing a metal-free core and peripheral oxygen donor sites, offers a unique platform for Cu^{2+} ion interaction.In the presence of Cu^{2+} ions, the free-base phthalocyanine structure is capable of forming coordination interactions through peripheral oxygen atoms, leading to the formation of more hydrophobic species.

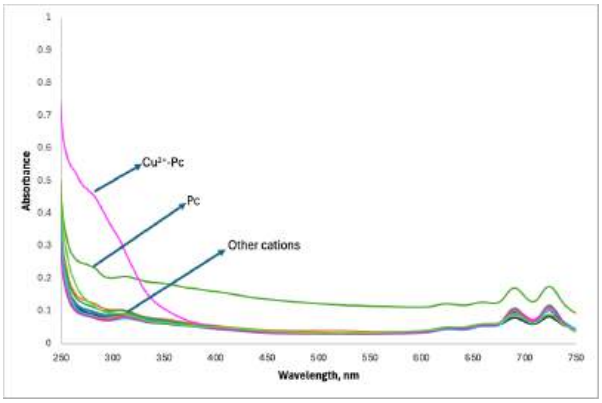

Fig. 1. UV–Vis absorption spectra of metal free phthalocyanine (Pc) at a concentration of 5×10^{-5} M, in the presence of Cu^{2+} ions and other metal cations added at tenfold excess

The development and optimization of the analytical method were carried out using a two-step chemometric approach. Initially, a Plackett–Burman design was employed to screen the main experimental variables affecting extraction efficiency, including ligand concentration, extraction solvent volume, disperser solvent volume, pH, centrifugation time, and centrifugation speed. Subsequently, the statistically significant factors were further optimized using Central Composite Design (CCD).
This work reports the first synthesis, characterization, and DLLME-based analytical application of a novel phthalocyanine derivative, highlighting the strong potential of chemometric-assisted microextraction strategies in metal ion determination and chemosensor development.

This work was supported by the TUBITAK 2209/A Research Support Program for Undergraduate Students.

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CCS - D2 - P05

Photocatalytic CO_2 reduction under visible light using ordered and disordered ceria–zirconia-based catalysts

Stjepan Šarić[1], Harshita Chawla[2], Dalibor Tatar[1], Jelena Kojčinović[1], Tina Skalar[3], Andreja Žgajnar Gotvajn[3], Marjan Marinšek[3], Matjaž Finšgar[4], András Sápi[2], Igor Djerdj[1]

[1]Dept. of Chemistry, Josip Juraj Strossmayer University of Osijek, Croatia; [2]Dept. of Applied and Environmental Chemistry, University of Szeged, Hungary; [3]Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia; [4]Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia

Cerium oxide (CeO_2) and mixed ceria-zirconia-based solid solutions have attracted substantial attention in the area of CO_2 hydrogenation in UV and visible light due to their high oxygen storage capacity (OSC) and the ability to effortlessly change its oxidation state. Following this knowledge, the high-entropy rare-earth counterparts were synthesized using the modified aqueous citrate sol-gel method.[1] We elucidate the structure transformation between ceria-zirconia based and its high-entropy counterparts, pyrochlore and kappa phases, by leveraging typical structural probes. The DRIFTS spectra showed that LCPGY compounds, especially partially oxidized *p*-LCPGY, consist of multiple oxygen vacancies and surface hydroxyl groups along with Ce and Pr centres, which are redox active through their reversible valence state changes. UV-Vis-NIR and XPS analysis showed that even though band gap values are more than 3 eV, these materials are visible light active due to multiple bandgaps owing to different metal cations, especially Ce and Pr. The photoreduction activity was investigated by photocatalytic hydrogenation of CO_2 in visible light. The results showed that all of the ceria-zirconia-based oxides and only the high-entropy solid solution (LCPGY) maintained selectivity just for CO, while the pyrochlore and partially oxidized pyrochlore forms of LCPGY produced 5.21% and 10.17% formaldehyde, respectively. The final results demonstrated that the highest CO_2 conversion was reached by *p*-LCPGY (24.14%), followed by partially oxidized *p*-LCPGY (21.76%) and κ-CeZrO (20.74%). An examination of the reaction progression shows that the inclusion of entropy effects not only promotes rapid CO_2 activation at early stages but also sustains catalytic activity throughout the process by stabilizing mixed-valence species. In contrast, κ-CeZrO illustrates how a highly ordered structure and balanced redox behavior contribute to improved long-term performance once the reaction reaches steady-state kinetics.

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CCS - D2 - P07
Redox-active ligand-driven oxygen evolution by molecular cobalt(III) catalyst

Dipanjana Sarkar[1], Sarita Yadav[2], Madhulika Gupta[2] and Ramesh K. Metre[2]
[1]Indian Institute of Technology Jodhpur, India; [2]Indian Institute of Technology Dhanbad, India

Efficient and stable molecular electrocatalysts based on earth-abundant metals are crucial for advancing sustainable energy technologies. We report the synthesis and detailed characterization of a mononuclear anionic cobalt (III) complex supported by a redox-active tridentate salicylaldiminate derivative of *o*-aminophenol. Spectroscopic techniques, complemented by single-crystal X-ray diffraction (SCXRD), confirm a distorted octahedral geometry around the cobalt centre, with additional stabilization in the solid state arising from weak C–H···O interactions.

Electrochemical studies using cyclic voltammetry in solution and in the solid state reveal quasi-reversible oxidation processes that are predominantly ligand-centered, highlighting the non-innocent behaviour of the aminophenol framework. The molecular complex was immobilized on a glassy carbon electrode and evaluated as an electrocatalyst for the oxygen evolution reaction (OER) in alkaline media (1.0 M KOH). The catalyst displays an onset potential of 1.56 V vs RHE and achieves a current density of 10 mA cm^{-2} at an overpotential of 410 mV. The favourable reaction kinetics are indicated by a low Tafel slope of 55 mV dec^{-1}.

Post-catalytic UV–visible, FT-IR, and X-ray photoelectron spectroscopy (XPS) analyses confirm the retention of molecular integrity after electrolysis, excluding catalyst degradation or conversion to cobalt oxide species. Density functional theory (DFT) calculations provide mechanistic insight into the catalytic process, revealing a ligand-centered water oxidation pathway facilitated by metal–ligand cooperativity. These findings emphasize the importance of redox-active ligand design in enabling efficient and durable molecular OER catalysis using first-row transition metals.

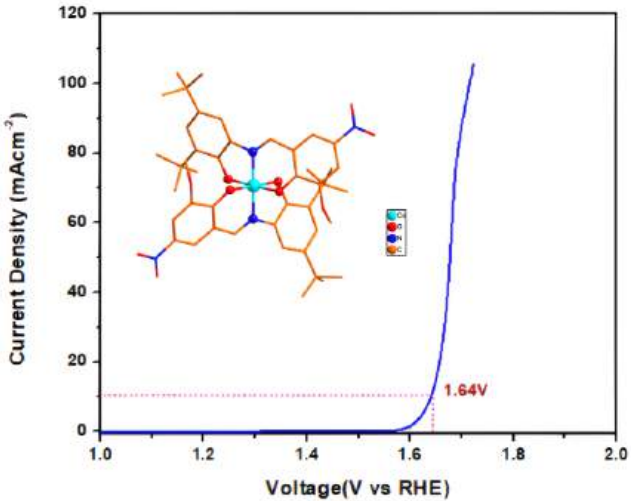

Fig. 1. Molecular cobalt(III) complex and its electrocatalytic performance towards oxygen evolution reaction

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CCS - D2 - P08

Cell-in-series testing as an accelerated tool for predicting performance and component degradation in flow batteries

Raphaël Delogne[1], Hao Yu[2], Luis Fernando Arenas[3], Jonas Hereiigers[4]
[1]Research Group Applied Electrochemistry & Catalysis, University of Antwerp, Belgium

Flow batteries (FBs) are promising candidates for large-scale energy storage due to their scalability, long cycle life, and decoupled power and energy capacities. A detailed understanding of the physical mechanisms driving capacity fade and component degradation is essential for accurate performance prediction[1]. However, this remains challenging because FBs are a complex system, containing multiple components interacting and evolving over time, affecting performance and durability.

Model-based state estimation methods for state of charge (SOC) and state of health (SOH) require extensive experimental validation, which is often time-consuming due to the large number of operational and design parameters influencing ageing and degradation, including temperature, cut-off voltage, current density, and electrolyte flow rate. [2]

To overcome these limitations, Accelerated Stress Tests (ASTs) have been developed to reproduce long-term cycling effects within shorter experimental timescales. ASTs may focus on individual components such as electrolytes, membranes, or electrodes or on the complete cell, for a better understanding of how operating conditions and material properties affect performance and lifetime.

Among these approaches, the Cell-in-Series (CIS) method, initially proposed by Pezeshki *et al*.[3] and later extended by our group[4], isolates degradation phenomena by operating two cells in series under controlled conditions, with one cell charging while the other discharges. This configuration enables precise monitoring of material and performance changes in a full cell assembly and facilitates the identification of operating conditions that significantly contribute to performance loss.

In this presentation work, we provide a detailed overview of the CIS methodology to rapidly identify optimal operating metrics for enhanced FB performance and durability.

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CCS - D2 - P09

From ion transport to electron storage: Rethinking the fundamentals of electrochemical energy storage

Hamed Pourzolfaghar[1], Yuan-Yao Li[1]
[1]Dept. of Chemical Engineering, National Chung Cheng University, Taiwan

Electrochemical energy storage technologies have progressed significantly, yet they remain fundamentally limited by ion-transport-dominated charge storage mechanisms. In conventional batteries and hybrid capacitors, energy storage relies on ion diffusion, insertion, or conversion within electrode materials, leading to restricted charging rates, structural degradation, and strong temperature dependence. These limitations are intrinsic to ion-centric mechanisms and persist across diverse electrochemical systems.

This work advocates a paradigm shift toward electron-dominant energy storage. By reconsidering electrochemical storage from the perspective of fundamental charge carriers, we emphasize the advantages of electrons, high mobility, minimal structural disruption, and reduced thermal sensitivity, as primary agents for reversible energy storage. Emerging strategies such as dielectric electron trapping, electrides with interstitial anionic electrons, electron-localized redox lattices, and surface-confined electron accumulation are discussed as pathways to bypass long-range ion transport.

Experimental approaches for validating electron-dominant behavior, including ion-blocking electrolytes, operando spectroscopy, and kinetic decoupling methods, are outlined. This electron-centric framework opens new opportunities for fast-charging, low-temperature, and solid-state energy storage systems, offering a foundation for next-generation technologies beyond the constraints of conventional ion transport.

Acknowledgment: The authors acknowledge financial support from the Ministry of Science and Technology (MOST), Taiwan (Grant No. NSTC 114-2221-E-194-002-MY3), and the Advanced Institute of Manufacturing with High-tech Innovations (AIM-HI) under the Higher Education Sprout Project of the Ministry of Education (MOE), Taiwan.

CCS - D2 - P10

From isoprene units to bioactive architectures: Mechanistic insights into isoprenoid biosynthesis

Hsiao-Ching Lin[1]

[1]Institute of Biological Chemistry, Academia Sinica, Taiwan

Isoprenoids constitute one of the most diverse families of natural products and underpin numerous medicinal and industrial applications. Built from five-carbon isoprene units derived from central metabolism, isoprenoids achieve remarkable structural and functional diversity through enzyme-catalyzed carbon-carbon bond formation, cyclization, and oxidative tailoring. Two particularly compelling features are the generation of complex core scaffolds and the site-selective activation of otherwise inert C–H bonds that enables downstream diversification. Our group focuses on discovering new bioactive, structurally complex isoprenoids and elucidating the enzymes and pathways responsible for their assembly and modification.[1–3] By defining the catalytic logic and mechanistic principles that govern scaffold construction and selective functionalization, these findings will expand the biosynthetic toolkit for natural product research and inspire new strategies for generating pharmacologically valuable molecules.

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CCS - D2 - P11
From furfural to 1,4-pentanediol, exploring an uncommon product of furfural hydrogenation

Vitaliy Masliy[1,2], Sreelakshmi Venugopalan[1,2], Eszter Baráth[1]
[1]Leibniz-Institut für Katalyse (e.V. LIKAT), Germany; [2]Univ Rennes, Institut des Sciences Chimiques de Rennes, France

In last decades, furfural gaining exponential scientific and industrial interest as a renewable, bio-based platform chemical. Nowadays, thousands of scientists work on this topic with hundreds of high impact papers are published each year. The most intensely researched furfural products are without a doubt the 2-methyltetrahydrofuran, γ-valerolactone and the levulinates.[1] Research around those chemicals gave birth to several commercially successful companies, such as transfurans Chemicals (Belgium), Lenzing AG (Austria), Pennakem LLC (USA), just to name a few. Although plenty of research have been done on furfural, some products remain obscure and undeveloped due to the complexity of the chemical cascade and humins/polymerization issues commonly observed during the reaction.[1] Some of the most commercially interesting products include 1,4-pentanediol and the cyclopentanol.[1,2] To the best of your knowledge, only a handful of publications describe the preparation of this compounds using furfural as starting material, and they mainly describe homemade catalysts which are difficult to employ at industrial scale.[2,3,4]
In this communication we described the preparation of 1,4-pentanediol in a cascade, one pot reaction. Commercially available ruthenium catalysts combined with commercial triflates were used. The screening included as Xantphos, triphenylphosphine, DPPE, DPPF, Ru-Macho, Triphos, BINAP and others. Unexpectedly, the best results were achieved under high concentration, when using BINAP and scandium triflate, yielding up to 45% of 1,4-pentanediol. The influence of the solvents, temperature and concentration will also be presented. Optimal conditions for other products are also presented in fewer detail, including cyclopentanol and 2-methyltetrahydrofuran. We also described the possible mechanisms and delve in to the challenges that come from this reaction and possible solutions.

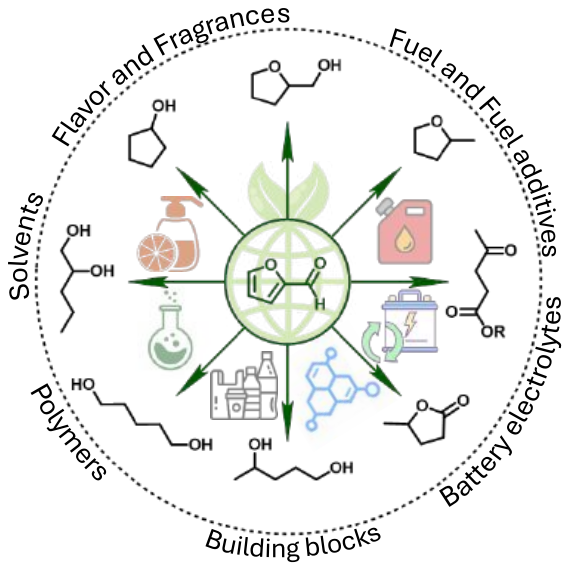

Fig. 1. Relevant furfural products and their possible applications

Acknowledgements: This work was performed with the of European Union Grant MSCA-DN-ChimSep GN: 101119277.

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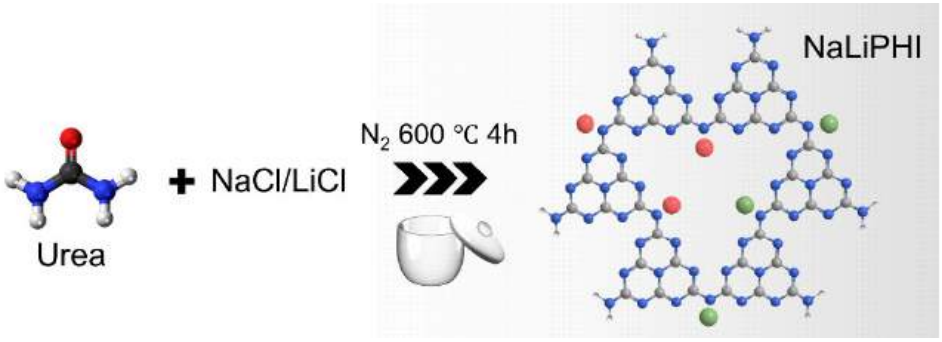
CCS - D2 - P12
Transforming ionic cocrystals into next-generation ionic carbon nitrides for solar fuel production

Anna Lo Presti[1], Christian Mark Pelicano[1], Markus Antonietti[1]
[1]Dept. of Colloid Chemistry, Max Planck Institute of Colloids and Interfaces, Germany

Solar-driven catalysis using particulate semiconductors represents a promising approach for the sustainable generation of valuable fuels. Poly(heptazine imide) (PHI), a new class of crystalline ionic carbon nitrides (CNs), has emerged as a standout photocatalyst due to its efficient visible-light absorption and optimal energy level alignment, which satisfy the requirements for driving hydrogen peroxide (H_2O_2) evolution. PHIs can be synthesized from N-rich compounds either using alkali metal chloride eutectic melts or through solid-state reactions involving alkali metal chlorides. They can also be prepared from pre-condensed covalent CNs by post-treatment with alkali metal salts.



Scheme 1. Fabrication of NaLiPHI from urea-LiCl/NaCl cocrystal.

Herein, we present an innovative strategy to unlock new ionic CNs by annealing ionic cocrystals (ICCs). These ICCs are formed through the solid-state association of neutral organic molecules with inorganic salts, particularly alkali and alkaline earth halides.[1, 2] We have identified a new PHI variant by pyrolizing a urea:LiCl:NaCl cocrystal (Sch. 1). This variant contains substantial amount of Li, which is unusual for benchmark KPHI and NaPHI catalysts. The optimal catalyst shows significantly improved H_2O_2 quantum efficiency (at 410 nm excitation wavelength)—up to threefold higher than conventional NaPHI. We are currently examining how the presence of Li affects the PHI framework. Additionally, we are exploring other ICCs derived from N-rich compounds and assessing their potential for diverse photocatalytic applications. Building on these insights, the unique interactions within ICCs present a promising pathway for creating ionic carbon nitrides (CNs) with innovative material properties and enhanced photocatalytic performance.

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CCS - D2 - P13
Titanocene-catalyzed hydrosilylation of oxetanes

Umut Kilic[1], Harie Goli[1], Stefan Grimme[2], Zheng-Wang Qu[2], Andreas Gansäuer[1]
[1]Kekulé-Institut für Organische Chemie und Biochemie, Germany; [2]Mulliken Center for Theoretical Chemistry, Germany

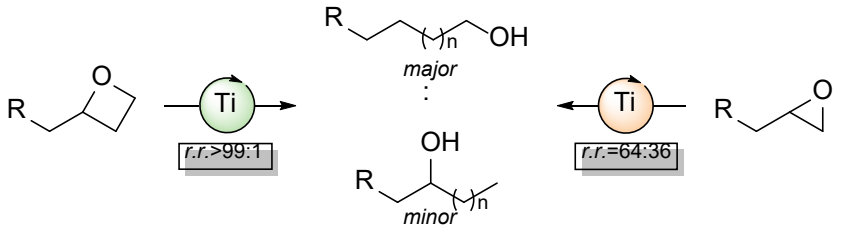
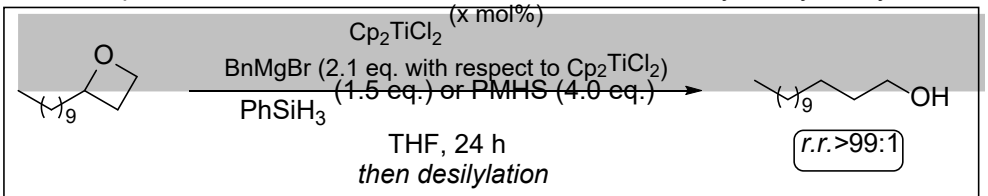


Fig. 1. Comparison of titanocene-catalyzed reductive ring opening of monosubstituted epoxides and oxetanes (*r.r.* = regioisomeric ratio).

The titanocene-catalyzed hydrosilylation proved to be a good method for the reductive ring opening of benzylic, allylic, and tertiary epoxides. However, its application to monosubstituted oxiranes is limited concerning the regioselectivity. In this work, we describe the use of oxetanes as promising alternative substrates to yield primary alcohols in high yields, under robust reaction conditions and with low catalyst loading. The transformation proceeds via single-electron transfer from the titanocene catalyst to the oxetane, followed by an intramolecular hydrogen atom transfer from the Ti–H species to the γ-titanoxy radical intermediate. Commercially available titanocene dichloride is employed as the catalyst, while $PhSiH_3$ or the inexpensive industrial waste product PMHS can be used as terminal reductant. Compared to epoxide hydrosilylation, the ring opening of oxetanes is more selective and sustainable. The difference in reactivity and selectivity was investigated and is rationalized by comparative DFT calculations.

Table 1. Optimized reaction conditions of the titanocene-catalyzed hydrosilylation of oxetanes.



cat. load	silane	temperature	conversion/%	yield/%
10 mol%	$PhSiH_3$	r.t.	99	85
5 mol%	$PhSiH_3$	reflux	100	85
1 mol%	$PhSiH_3$	reflux	100	78
1 mol%	PMHS	reflux	100	75

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CCS - D2 - P14

Discovery of new catalysts for the radical arylation reaction by predictor-based cyclic voltammetry (CV) screening

Lennart Hanz[1], Niklas Schmickler[1], Sergei Gerber[1], Stefan Grimme[2], Zheng-Wang Qu[2], Inke Siewert[3], A. Gansäuer[1]

[1]*Keklulé Institut für Organische Chemie und Biochemie, Universität Bonn, Germany;* [2]*Mulliken Center for Theoretical Chemistry, Universität Bonn, Germany;* [3]*Institut für Anorganische Chemie, Georg-August-Universität Göttingen, Germany*

The radical arylation reaction with titanocene halides suffers mainly from two aspects. Firstly, electron poor titanocenes are required to facilitate the rate determining step of the reaction.[1] This requires additional synthetic effort to modify the electronic properties of the titanocene complexes for substrates with electron-deficient arenes. The second aspect is the requirement of halide abstracting supramolecular H-bond donors especially during electrochemical reduction of titanocene halides.[2] Cyclic voltammetry can visualize these properties in the form of peak potentials for the different species that are present during catalysis. These peak-potentials as well as the position of the E_qC_r equilibrium[2] can be used as predictors for the efficiency of catalysis for this system. Our CV screening, by employing those predictors, is advantageous to classical methods, since only the catalysts are required, saving time and resources. This makes the whole process more sustainable and more efficient.

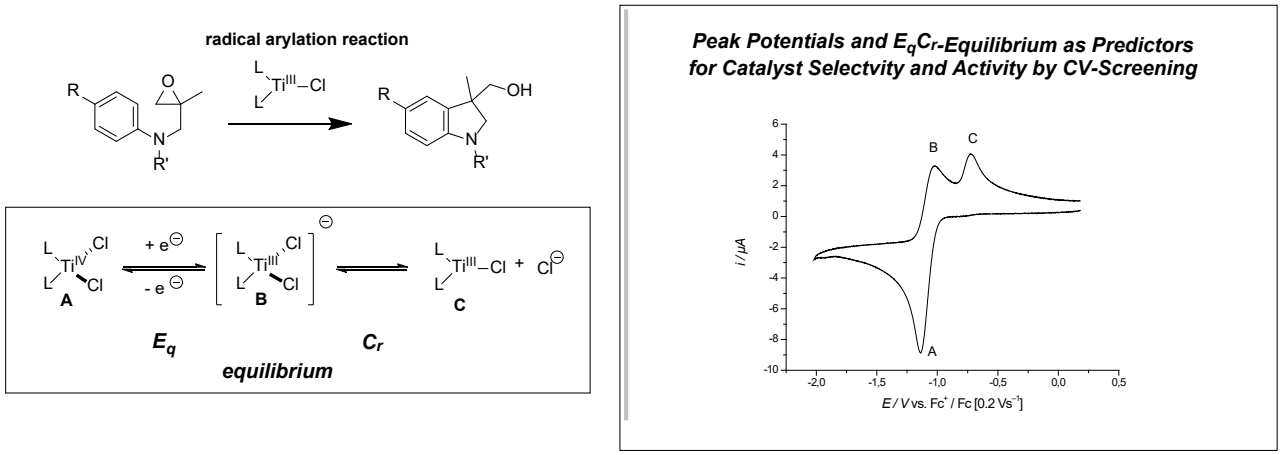

Fig. 1. Predictor–based CV-screening approach for the radical arylation reaction.[3]

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CCS - D2 - P15

Carboxylic acid-based carbon-carbon cross-coupling by radical decarboxylation's in continuous flow

Cathal Kelly[1], Carl Mallia[2], Marcus Baumann[1]
[1]University College Dublin, Ireland; [2]AstraZeneca, UK

Finding a more efficient, cost-effective way of achieving carbon–carbon cross-coupling to access C(sp^2)–C(sp^3) compounds is in high demand for the pharmaceutical industry.[1] Incorporating cheaper and more abundant starting materials and earth-abundant metals has the potential to deliver substantial benefits. Carboxylic acids are abundant, stable, and inexpensive feedstocks, but their direct use as carbon nucleophiles in C(sp^2)–C(sp^3) bond formation remains challenging under mild and scalable conditions. This work presents a continuous flow process for carbon-carbon coupling that leverages radical decarboxylation of carboxylic acids (via redox-active ester activation) to generate alkyl radicals, which engage in nickel-catalysed coupling with a range of vinyl halide electrophiles. Exploitation of nickel catalysis and a zinc packed-bed column provide a cost-effective alternative to existing methods accessing sp^2–sp^3 coupled compounds, avoiding the use of expensive photocatalysts and rare earth metals.[2] This work has currently achieved successful coupling of a range of secondary and tertiary radicals with electrophilic vinyl halide partners in moderate yields. This flow-enabled decarboxylative cross-coupling offers a practical approach to transform simple carboxylic acids building blocks into valuable chemical compounds, with enhanced operational safety and scalability relative to batch radical processes.

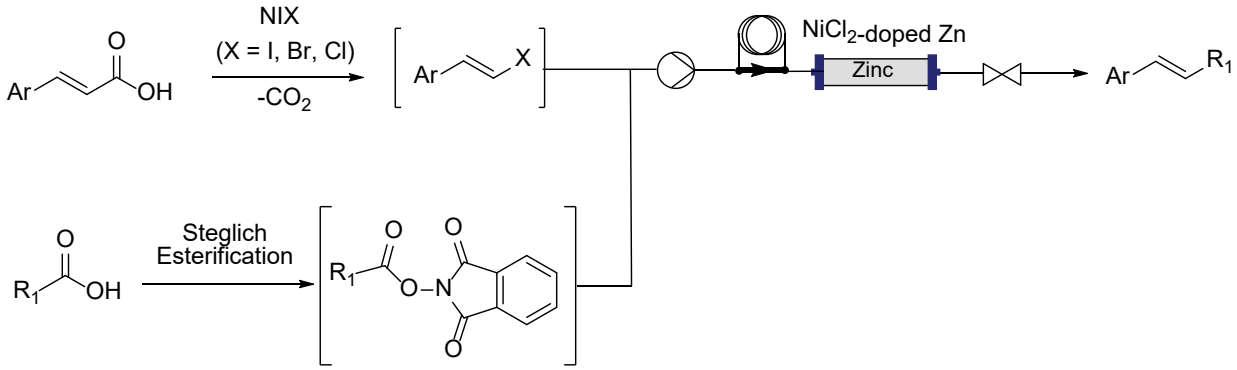

Fig. 1. Radical mediated C-C cross-coupling in continuous flow

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CCS - D2 - P16

Electrochemical conversion of kenaf biomass to glucose: Role of reactive chlorine species on dimensionally stable anodes

Ji Yeon Park[1], Jin Hyng Lee[1]
[1]Korea Institute of Ceramic Engineering and Technology, Rep. Korea

Electrochemical hydrolysis has gained increasing attention as an enzyme-free and environmentally benign approach for lignocellulosic biomass conversion. Despite its promise, the chemical factors governing polysaccharide depolymerization under electrochemical conditions remain poorly understood. This study investigates the role of electrochemically generated reactive chlorine species (RCS) in the conversion of kenaf biomass to glucose using dimesionally stable anode (DSA)-type mixed metal oxide electrodes.

Distinct saccharification behavior observed under RCS-active and RCS-suppressed electrochemical environments demonstrates that RCS play a decisive role in promoting glycosidic bond cleavage. The results indicate that chlorine-derived reactive intermediates significantly enhance biomass deconstruction beyond conventional acid-driven pathways, highlighting the unique reactivity enabled by DSA-based electrochemical systems. Rather than relying on enzymatic catalysis, the process leverages electrochemically induced reaction environments to facilitate efficient carbohydrate release from lignocellulosic structures.

Overall, this work establishes a clear conceptual link between RCS activity and enhanced electrochemical saccharification, providing new insight into chlorine-mediated reaction pathways in biomass conversion. The findings position electrochemical hydrolysis using DSA-type electrodes as a promising and scalable platform for sustainable biomass valorization and green chemical processing of renewable resources.

CCS - D2 - P17

Density functional theory exploration of Mo_3S_4 cluster-catalyzed phenyl acetylene hydrogenation in the presence of acrylonitrile

Vicent S. Safont[1], Rosa Llusar[1], Mónica Oliva[1], Juanjo Mateu-Campos[1], Juan Andrés[1]
[1]Universitat Jaume I, Spain

We have recently reported[1] an unprecedent C-C cross coupling reaction via the generation of benzyl radicals from terminal aromatic alkynes along their hydrogenation processes. The reported protocol employed diamino Mo_3S_4 cubane-type clusters as catalysts. A sulfur-centered cluster catalysis mechanism was proposed for the radical formation, based on catalytic and stoichiometric experiments.

In the present contribution we present theoretical calculations at the state-of-the-art DFT level on the phenyl acetylene hydrogenation catalyzed by $[Mo_3S_4Cl_3(dmen)_3]^+$ (dmen=N,N'-dimethyl-ethylenediamine) cluster in the presence of acrylonitrile as radical acceptor. Two reaction pathways, one leading to styrene and the other rendering the benzyl radical, that experiences a Giese-type addition reaction with the acrylonitrile to form 4-phenylpentanenitrile, have been characterized, in accordance with the observed outcome of the reaction.

It has been found that several Hydrogen Atom Transfer (HAT) processes take place with associated spin changes from singlet to triplet (or doublet, for the radical species) states and *vice versa*. We have previously found[2] this kind of behavior in the selective semi hydrogenation of internal alkynes, catalyzed by Mo_3S_4 imidazolyl amino clusters.

As experimentally suggested, both reaction pathways begin with the cluster hydrogen activation to form a bis(hydrosulfide) intermediate. This intermediate can react with the alkyne via two consecutive HATs to render styrene. Conversely, the intermediate can experience several HATs and further hydrogenation processes when interacting with the phenyl acetylene, making possible the formation of the benzyl radical that reacts with acrylonitrile to form the 4-phenylpentanenitrile, see Figure 1. Our results further support the proposed mechanism and renders a detailed description of the process.

Fig. 1. Schematic representation of the reaction pathways for the phenyl acetylene hydrogenation catalyzed by $[Mo_3S_4Cl_3(dmen)_3]^+$ in the presence of acrylonitrile.

The financial support from the Spanish Ministerio de Ciencia e Innovación (PID2022-141089NB-I00) and Generalitat Valenciana (CIAICO/2024/94) is greatfully acknowledged.

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CCS - D2 - P18
Perovskite-type lanthanum cobalt oxide powders synthesized by reactive milling

Serhii Tkachenko[1], Vendula Bednaříková[1], Michaela Remešová[1], Martina Vrankić[2], Melita Menelaou[3], Ladislav Čelko[1]
[1]Central European Institute of Technology, Brno University of Technology, Czech Republic; [2]Ruđer Bošković Institute, Croatia; [3]Cyprus University of Technology, Cyprus

The use of reactive milling to synthesize catalytically active powders, including lanthanum cobaltite perovskite ($LaCoO_3$), has attracted considerable interest. This approach provides an environmentally friendly, solvent-free, and scalable synthesis route, offering high-yield and clear advantages over conventional solution-mediated methods. In this study, a two-step top-down reactive milling process was investigated to synthesize $LaCoO_3$ perovskite powder. The synthesis employed high-energy mechanical activation of lanthanum(III) oxide (La_2O_3) and ($Co(OH)_2$) via planetary ball milling or horizontal attrition, followed by a solid-state reaction triggered by thermal calcination in air. The structural, morphological, and surface properties of the resulting powders – along with the progression of mechanochemical and solid-state reactions leading to $LaCoO_3$ formation – were characterized using high-resolution scanning electron microscopy (HR-SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Brunauer–Emmett–Teller (BET) surface area analysis. The results showed that reactive milling of the precursor powders in a horizontal attritor enables the direct formation of $LaCoO_3$ and improves reactivity towards subsequent solid-state reactions, yielding nearly single-phase $LaCoO_3$ at calcination temperatures as low as 650 °C. In contrast, powders mechanically activated using a planetary ball mill exhibited $LaCoO_3$ formation only during calcination and required substantially higher calcination temperatures (850-1050 °C) to achieve acceptable phase purity.

The authors acknowledge the CLiCAM project (HORIZON-WIDERA-2022-TALENTS-03-01 programme, Grant No. 101120555) for financial support of the research. Authors also acknowledge the CzechNanoLab Research Infrastructure, supported by the Ministry of Education, Youth and Sport of the Czech Republic (LM2023051), for providing access to the equipment used in this study. Zoz GmbH is gratefully acknowledged for providing the necessary equipment and technical expertise for the reactive milling experiments.

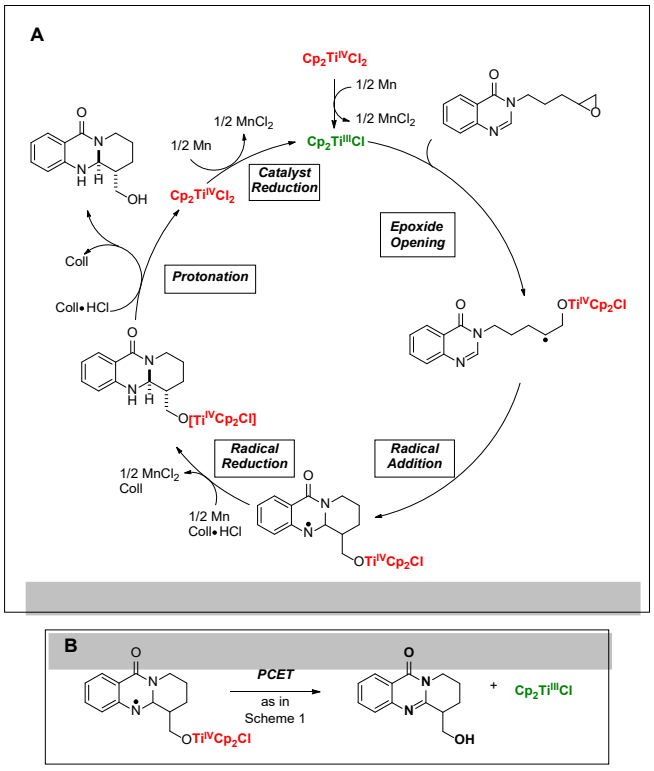
CCS - D2 - P19

Dihydroquinazolinones by titanocene catalyzed reductive radical addition to quinazolinones

Konstantin Woitol[1], Thomas Heinrichs[1], Andreas Gansäuer*[1]

[1]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Germany

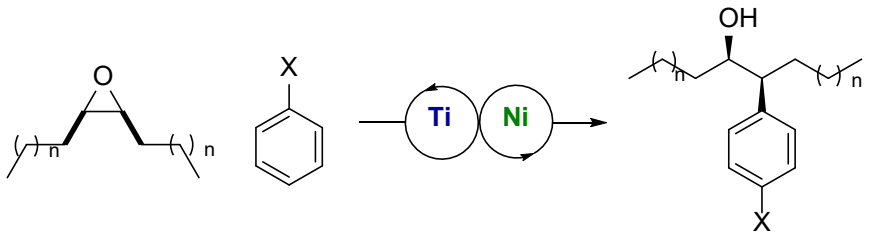
We report a novel titanocene-catalyzed approach to functionalized dihydroquinazolinones via intramolecular radical addition. The reaction relies on an unusual reduction of the radical σ-complex formed upon addition of an epoxide-derived β-titanoxy radical, a step not previously reported in titanocene-catalyzed radical arylations. The reaction proceeds with high diastereoselectivity and accommodates a broad range of functional groups at the pharmaceutically important 6- and 7-positions of the dihydroquinazolinone scaffold. Subsequent oxidation of the products to the corresponding quinazolinones can be achieved using MnO_2.



CCS - D2 - P20
Cross elecrophile coupling of unstabilzed epoxides by Ni&Ti cooperative catalysis

Niklas Schmidt[1], Andreas Gansäuer[2]
[1]University of Bonn, Germany

Non-stabilized (non-bicyclic, non-benzylic) epoxides are converted to *β*-aryl alcohols in high enantioselectivities and moderate diastereoselectivities. This expands the sope of the current cross-electrophile couplings which are limitated to the coupling of cyclic[1] or benzylic[2] radicals. Chiral Titanocene catalysts are responsible for controlling both enantio- as well as diastereoselectivity.



up to 88% yield
98% *ee*
d.r. = 85:15

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CCS - D2 - P21

Conversion of CH_4 and CO_2 into acetic acid: The potential of montmorillonite as a catalyst

Gabriel Lopes[1], Alessandra Lucrédio[1], Luiz H. Vieira[1], Teresa Blasco[2], Elisabete Assaf[1]
[1]São Carlos Institute of Chemistry, University of São Paulo, Brazil; [2]Institute of Chemical Technology, Polytechnic University of Valencia, Spain

The emission of greenhouse gases (CO_2 and CH_4) is one of the main factors driving climate change,[1] and the valorization of these gases has emerged as a promising alternative,[2] despite their high thermodynamic stability.[3] Acetic acid is produced by processes such as Monsanto and Cativa.[4] The synthesis of acetic acid via heterogeneous catalysis has been explored. Montmorillonite (MMT), stands out as a sustainable catalytic support.[5] The catalytic potential of MMT in the direct conversion of CH_4 and CO_2 into acetic acid was investigated. The commercial MMT K-10, previously calcined at 700 °C, was subjected to a reduction treatment under a pure H_2 flow of 30 mL.min^{-1} with a programmed heating rate of 10 °C.min^{-1} to 545 °C. Catalytic activity was evaluated in a batch reactor. 500 mg of the calcined and reduced material was pretreated at 300 °C under an N_2 flow, and the reactions were carried out at 2 and 6 bar using an equimolar CH_4/CO_2 mixture, under stirring at 600 rpm for 5 h. After the reaction, the reaction products were extracted from the catalyst with deionized water. The extract was analyzed by HPLC. In addition to TPR-H_2, EDS was performed to determine the chemical composition of the material. The catalytic tests showed no activity for calcined MMT K-10, regardless of the pressure evaluated. The reduced material exhibited acetic acid productivities of 153 and 178 μmol.g^{-1}.h^{-1} at 2 and 6 bar, respectively. TPR-H_2 analysis (Fig. 1a) revealed multiple reduction events associated with Fe species.[6] The natural presence of Fe and K was confirmed by EDS (Fig. 1b), with homogeneous distribution within the MMT structure.[7] These results indicate that, after reduction, Fe-related active sites become accessible, favoring CH_4 activation, while K contributes to CO_2 adsorption due to its basicity, imparting a bifunctional catalytic character to the reduced MMT K-10.

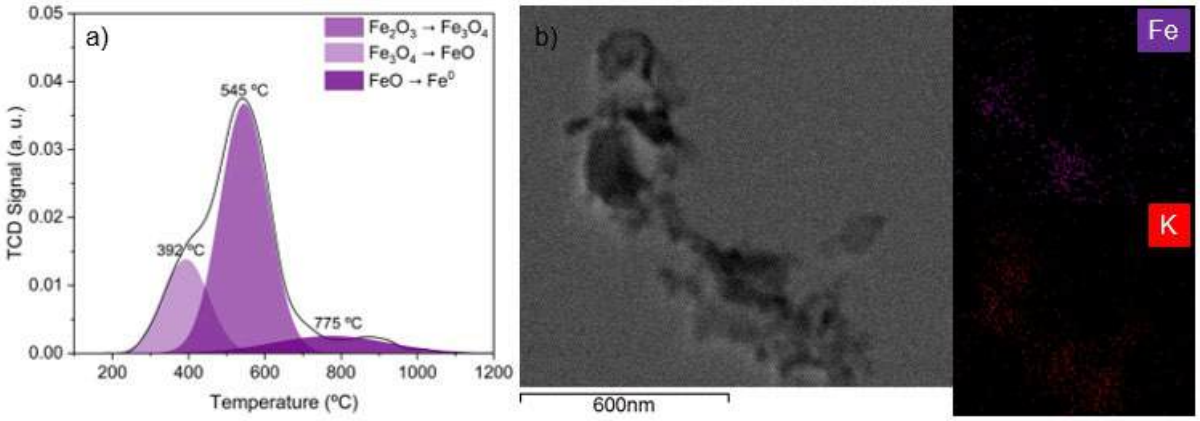

Fig.1. a) Temperature-programmed reduction (TPR-H_2) profile; b) EDS analysis evidencing the presence of iron and potassium in the clay.

The authors are grateful for the financial support of the São Paulo Research Foundation (FAPESP) (Projects: 2025/24688-9, 2024/04540-4, 2022/06419-2, and 2022/10615-1) and the National Council for Scientific and Technological Development (CNPq) (Project: 300454/2025-2).

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CCS - D2 - P22
Copper(II)-based metal-organic materials as catalysts for the hydrogen evolution reaction

Claire Bradley[1,2], Athira Ravi[1,2,3], Joseph Eiffe[1,2], Gearóid Manning[1,2], Sebastien Vaesen[1,2], Nianyong Zhu[1,2], Wolfgang Schmitt[1,2,3]
[1]School of Chemistry, Trinity College Dublin, Ireland; [2]Centre for Research on Adaptive Nanostructures and Nanodevices & AMBER, Trinity College Dublin, Ireland; [3]SSPC, University of Limerick, Ireland

Coordination cages and metal-organic frameworks (MOFs) are supramolecular materials known for their adjustable pore sizes, tuneable structures and exceptionally high surface areas, rendering them attractive platforms for catalysis, gas storage and separation technologies.[1, 2] This work investigates copper(II)-based coordination cages and MOFs as electrocatalysts for the hydrogen evolution reaction (HER). Hydrogen, a non-carbon fuel with the highest gravimetric energy density, is a promising solution to the global energy crisis. However, high preparation costs and need for expensive, rare-earth catalysts limit its widespread production. We report the synthesis of several copper(II) paddlewheel-based materials constructed from the previously reported 3,3',3''-(1,3,5-triyl)tris(ethyne-2,1-diyl)tribenzoate ligand and its amino-functionalised analogue,[3] affording isostructural nanoscopic cages: **Cu_{12}** and **$Cu_{12\text{-}NH2}$**, **Cu_{36}** and **$Cu_{36\text{-}NH2}$**, and the MOF: **MOF-$Cu_{36\text{-}NH2}$** which contains **$Cu_{36\text{-}NH2}$** cages connected *via* azopyridine linkers (Figure 1). The synthesised assemblies showed significant electrocatalytic activities for HER under near-neutral pH conditions. A notable increase in activity was observed in the amino-functionalised cages: **$Cu_{12\text{-}NH2}$** and **$Cu_{36\text{-}NH2}$**, attributed to beneficial electronic effects of the amine group. **$Cu_{36\text{-}NH2}$** showed the highest activity, achieving an overpotential of $\eta_{(10mAcm^{-2})}$=175 mV and Tafel slope of 115 mV/dec. All cages outperformed **MOF-$Cu_{36\text{-}NH2}$**, consistent with greater accessibility of copper active-sites in the discrete cages relative to the MOF. These results highlight copper coordination cages as promising, tuneable electrocatalysts for sustainable hydrogen production.

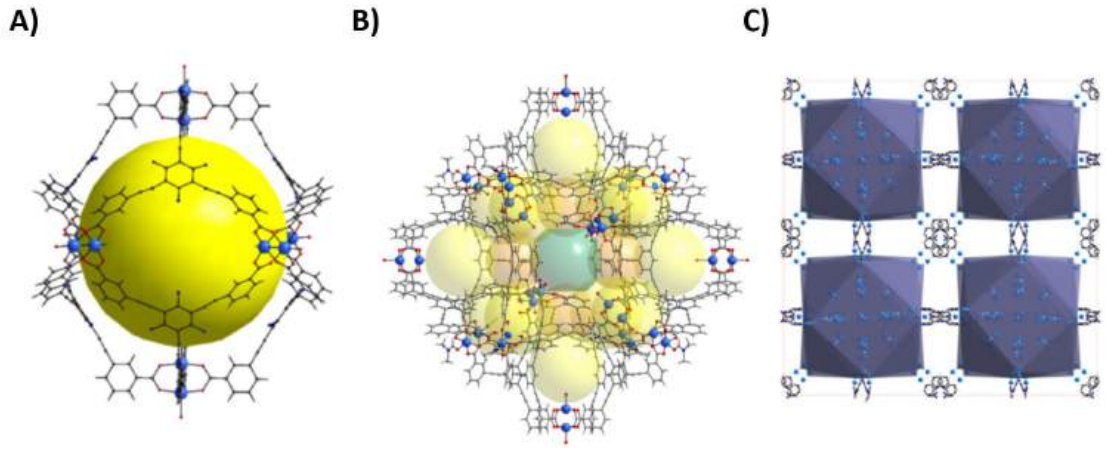

Fig. 2. Crystal structures of copper(II) based metal-organic materials. A) Cu_{12} and $Cu_{12\text{-}NH2}$, B) Cu_{36} and $Cu_{36\text{-}NH2}$ and C) MOF-$Cu_{36\text{-}NH2}$ (for A & B inner pores highlighted as spheres; C polyhedral representation)

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CCS - D2 - P23
Tuning heterogeneous catalysts for the depolymerization of polyurethane waste

Matilde Onofri[1], Jan Romano-de-Gea[1], Andras Bodi[2], Patrick Hemberger[2], Paul J. Dyson[1]
[1]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland; [2]Paul Scherrer Institute (PSI), Switzerland

As the constantly growing accumulation of plastic waste has resulted in an increasingly urgent environmental challenge, strategies for the recycling of end-of-life plastic products must be developed and implemented.[1] This work aims to investigate sustainable catalytic pathways for the chemical recycling of high-volume polymeric materials, specifically focusing on the recovery of the starting monomers from durable plastics through catalytic depolymerization strategies. Amongst these target materials, polyurethanes (PUs) are a versatile class of synthetic polymers whose broad applications include elastomers, coatings, flexible and rigid foams, adhesives, electrical encapsulating compounds, and fibres.[2] PUs (aromatic or aliphatic, thermoplastic or thermoset) are synthesized from isocyanates and polyols. However, the efficient recovery of the monomers from PU waste through industrially viable pathways remains under-investigated. In this work, heterogeneously catalyzed PU hydrogenolysis to the diamine and polyol constituents is investigated. Depolymerization tests on thermoplastic PU granules achieved high conversions (up to 97%) and significant monomers recovery (81% diamine, 80% diol) in optimized reaction conditions under molecular H_2. The most active catalyst maintained its performance over several reaction cycles and was able to depolymerize both flexible and rigid PU foams from real scraps to the corresponding constituent units, demonstrating the potential industrial use of the catalytic system for chemical recycling of PU waste.

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CCS - D2 - P24

Efficient catalytic hydrogenolysis of glycerol to 1,2-propanediol using a selective multifunctional nanotube-supported catalyst for developing a SMART multiphase reactor

Jakob Albert[1], Bodo Fiedler[2], Mirko Skiborowski[2]
[1]University of Hamburg, Germany; [2]Hamburg University of Technology, Germany

The fundamental principles of chemical reactors have changed little over the past century. However, the transition from fossil-based feedstocks to sustainable raw materials, which often exhibit significant variability in composition, poses a major challenge in reaction engineering. The Collaborative Research Center (CRC) 1615 “SMART Reactors” addresses this challenge by focusing on the development of advanced chemical and biotechnological reactors, as well as their components, to enable efficient adaptation to these new demands. Within the framework of the CRC, the hydrogenolysis of glycerol to 1,2-propanediol is studied as a multiphasic model reaction, which can be both chemically or biochemically catalyzed. A key focus of the chemically catalyzed process is the use of selective multifunctional catalysts that can be flexibly activated and deactivated. One approach to achieve this is leveraging carbon nanotubes (CNT) as support materials to tailor the catalytic properties of the catalyst. Based on previous investigations regarding the composition of the CNT-supported catalyst,[1] we have performed a detailed kinetic study for the heterogeneously-catalysed glycerol hydrogenolysis reaction using a multifunctional Ru-Cu catalyst in a slurry batch reactor system. These investigations examined the effects of critical parameters such as glycerol concentration, hydrogen saturation concentration, catalyst loading, reaction temperature, and gas flow rate on both the reaction kinetics and the overall process efficiency. These insights not only deepen the understanding of the hydrogenolysis reaction mechanism but also provide a foundation for optimizing catalyst design and reactor operation within the framework of SMART Reactors to maximize the yield and selectivity towards 1,2-propanediol.

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CCS - D2 - P25
Alternative mechanochemical route for producing silver powder from silver salts

Marcela Achimovičová[1], Dáša Drenčaková[1,2], Matej Baláž[1], Jaroslav Briančin[1], Maksym Lisnichuk[3], Mária Bali Hudáková[1], Lenka Hagarová[1]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia; [2]Faculty of Materials, Metallurgy and Recycling, Technical University of Košice, Slovakia; [3]Faculty of Science, Pavol Jozef Šafárik University Košice, Slovakia

Silver powder, produced in diverse nano-to microscale forms, is valued for its conductivity, antibacterial activity, and catalytic performance, enabling applications in electronics, antimicrobial materials, catalysis, and decorative products. Commercial synthesis relies mainly on liquid-phase chemical reduction of $AgNO_3$ with formaldehyde[1], while other methods[2-4] are generally less simple or environmentally favourable. The work focuses on novel alternative mechanochemical preparation of silver powder-nanoparticles from inexpensive and readily available precursors, various silver salts, by milling using iron powder as a reductant. Also, input silver precursors, namely silver sulfate and silver acetate, were used in these chemical reactions for the first time. The study includes monitoring the kinetics of the designed mechanochemical reactions, assessing the phase purity of the Ag products by X-ray diffraction, evaluating washing procedures, analysing elemental composition, examining Ag products' morphology using scanning and transmission electron microscopy, along with measurements of their specific surface area and particle size distribution. The time for Ag mechanochemical synthesis requires only 90 min. In addition to metallic silver powders, ferrous salts are formed as secondary products; their aqueous solutions can be utilised in various industrial and practical applications. The overall process is safe, simple, waste-free, and readily scalable for large-scale production.

Acknowledgements: This work was realised within the Slovak Grant Agency (VEGA 02/0036/23) and the Slovak Research and Development Agency under the contract No. APVV-24-0353.

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CCS - D3 - P01

Effect of non-metal dopants in self-coupled g-C_3N_4 Van der Waals heterojunctions for efficient photocatalytic tetracycline and PFOA degradation

Tim Jähnichen[1], James A Sullivan[1]
University College Dublin, Ireland

Most water treatment applications cannot fully remove Persistent Organic Pollutants (POP) such as antibiotics, microplastics, or per- and fluoroalkyl substances in wastewater streams, leading to their eventual accumulation in water sources and soils. This poses major risks to human health, e.g. due to the evolution of antibiotic-resistant bacteria or the ingestion and build-up of persistent pollutants in the body.[1] A sustainable and affordable method to degrade POP from wastewater is photocatalysis. Photocatalysts effectively harness solar energy to drive pollutant degradation by radical formation and reaction.[2] To date, many photocatalytic systems are based on rare and expensive (noble) metals or are unable to generate sufficiently oxidizing radicals due to their electronic characteristics. To overcome these challenges, our work focuses on synthesizing metal-free self-coupled g-C_3N_4 heterojunctions using an affordable melamine thermal polymerization method with different non-metal dopants. Self-coupled heterojunction formation between pristine and doped g-C_3N_4 is achieved by electrostatic self-assembly. Thereby, Z-scheme systems are formed that can greatly improve light utilization and charge-carrier separation compared to the component materials.[3] The photocatalytic performance of the synthesized materials is investigated for degradation of tetracycline (10 ppm) and perfluorooctanoic acid (PFOA, 100 ppm) as model compounds under simulated sunlight. During these experiments, the effect of different non-metal dopants, the dopant loading, and the ratio of component materials during heterojunction formation is analysed. We show that the photocatalytic activity of g-C_3N_4 photocatalysts is greatly improved compared to the component materials without the need for expensive metal doping.

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CCS - D3 - P02

NiX/Al_2O_3 catalysts for photocatalytic hydrogen production towards intended industrial application

Judit Lloreda[1,2], Jarosław Serafin[3], Xavier Vendrell[3], Vanessa Abad[2], Elvira Gómez[1], Albert Serrà[1]
[1]Thin-film and Nanostructure Electrodeposition Group (GE-CPN) – Universitat de Barcelona, Spain; [2]Consorci per a la Gestió dels Residus del Vallès Oriental, Spain; [3]Solid-state Chemistry Group (QES), Dept. of Inorganic and Organic Chemistry and Institute of Nanoscience and Nanotechnology (IN2UB) – Universitat de Barcelona, Spain

The increasing interest towards renewable feedstocks as green energy sources drives the development of new technological solutions. Hydrogen is an integral part of this sustainable chain, either as a fuel, a chemical reagent, or both. However, its large-scale production still relies mainly on fossil fuels. Photocatalytic production of hydrogen provides an environmentally friendly pathway, which also benefits from bioavailable oxygenated organic species such as ethanol. In any case, catalysts are required to operate under mild conditions and reduce energy costs. Nickel-based catalysts supported on aluminum oxide are a key technological platform for sustainable decarbonization, processes, including hydrogen production, thanks to their moderate cost, good metal dispersion and high thermal stability.
In this study, NiX/Al_2O_3 catalysts, where X = Ø, Cu, Fe or Co, were prepared by a standard wet impregnation method[1] using different metal ratios, while maintaining a constant total metal loading. SEM characterization prior to reaction confirmed the formation of nanoparticles of the active metals on the micrometric Al_2O_3 surface, as well as their homogeneous distribution. The materials were tested for photocatalytic hydrogen production, under 365 nm irradiation at room temperature. Argon was used as the carrier gas, flowing through a Dreschel bottle containing a 9:1 EtOH:H_2O mixture. Of all prepared catalysts, only the Ni-Cu bimetallic system showed H_2 production, which is attributed to the photoactivity of copper oxides. To confirm this behavior, Cu/Al_2O_3 was used as a reference material, while three different Ni/Cu ratios were also tested to evaluate the role of Ni. The $5Ni5Cu/Al_2O_3$ catalyst showed the highest hydrogen production, exceeding that of Cu/Al_2O_3. Finally, stability was assessed, under constant irradiation conditions and during light on/off cyclic experiments. These results highlight the relevance of $Ni\text{-}Cu/Al_2O_3$ catalysts under mild photocatalytic conditions.

Acknowledgements: With the support of the Industrial Doctorates Program of the Dept. of Research and Universities of the Generalitat de Catalunya (project 2022 DI 00035). The authors acknowledge financial support through the AGAUR grant (project 2023 CLIMA 00009), supported by the Dept. of Research and Universities, the Dept. of Climate Action, Food and Rural Agenda, and the Climate Fund of the Generalitat de Catalunya. The authors would also like to thank the CCiT-UB for the use of their equipment.

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CCS - D3 - P03

Heterogeneous catalysts synthesis by electroless deposition for environmental applications

Judit Lloreda[1,2], Vanessa Abad[2], Elvira Gómez[1], Albert Serrà[1]

[1]Thin-film and Nanostructure Electrodeposition Group (GE-CPN) – Universitat de Barcelona, Spain; [2]Consorci per a la Gestió dels Residus del Vallès Oriental, Spain

The development of nanocatalysts greatly benefit heterogeneous catalysis. The synthesis of metallic nanoparticles (NPs) on supports with large surface areas results in a well-dispersed high density of actives sites, thereby enhancing the catalytic activity. Achieving optimal catalytic performance requires precise control over the synthesis process to regulate the metal loading and dispersion. In this regard, electroless deposition enables accurate control over particle size and morphology while allowing metal deposition on a wide variety of supports. The typical composition of an electroless bath contains a metal precursor salt, complexing agents and a reducing agent, all balanced to sustain an efficient autocatalytic reaction[1]. Common reducing agents include phosphates and boranes, whose oxidation often results in the co-deposition of P or B heteroatoms, which may hinder the desired catalytic effect. To avoid this undesired incorporation, hydrazine is used, as its oxidation results in a complete decomposition into H_2 and N_2.

In this work, a Ru and a Ni electroless baths with hydrazine were used to prepare the catalytic materials using carbon-based supports. Regarding Ru bath[2], an optimization study was performed over fluorine-doped tin oxide coated glass (FTO) substrates and followed by UV-vis spectrophotometry. The thin films obtained were characterized by SEM microscopy coupled to EDS, to assess the deposition conditions. Using two carbon substrates, graphite flakes and carbon nanotubes (CNTs) a series of samples at different deposition times were prepared and morphological and compositionally characterized. Prior were successfully oxidized following an acid attack etching combined with ultrafast sonication, to reduce hydrophobicity and facilitate disaggregation, step that subsequently improved the necessary sensitization treatment with Sn and Pd. Optimal deposition conditions were established at 60 and 10 min for Ru and Ni, respectively. The suitability of the prepared materials as catalysts for methane decomposition reaction is currently under evaluation.

Acknowledgements: With the support of the Industrial Doctorates Program of the Dept. of Research and Universities of the Generalitat de Catalunya (project 2022 DI 00035). The authors would like to thank the CCiT-UB for the use of their equipment.

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CCS - D3 - P04

Amino acids as organocatalysts for the electrosynthesis of pinacols from 4-fluoroacetophenone

Claudiu Bostan[1], Martina Bortolami[1], Cristiana Margarita[1], Fabrizio Vetica[2], Marta Feroci[1]

[1]Dept. of Basic and Applied Sciences for Engineering (SBAI), Sapienza University of Rome, Italy; [2]Dept. of Chemistry, Sapienza University of Rome, Italy

The growing demand for chiral molecules drives the need for sustainable asymmetric synthesis. Electrosynthesis offers a promising green alternative to classical methods, utilizing selective redox reactions and atom economy to eliminate the need for stoichiometric mediators[1]. The electrochemical reduction of acetophenones is a well-known reaction that can yield either the corresponding alcohol or the dimerization product[2]. This work focuses on the electrochemical dimerization of acetophenones to pinacols. This pathway is particularly challenging compared to alcohol formation, as it requires dual stereoselective control: simultaneous enantioselection and diastereoselection.

To achieve precise stereocontrol, we investigated electrode functionalization via electrografting of microwave-synthesized chiral nanoparticles (L-Pro-NPs) or amino acids, alongside the use of free chiral amino acids in solution.. The successful modification of the Glassy Carbon electrode was confirmed by cyclic voltammetry, as detailed in Figure 1. Specifically, functionalization with chiral nanoparticles enhanced conductivity, whereas the L-Proline layer acted as an insulator, resulting in a marked current peak decrease. Subsequently, comparative electrosyntheses were conducted to optimize the process (results in Table 1), allowing us to reach yields up to 93% with significant variations in diastereomeric ratios.

We achieved exceptional yields and diastereoisomeric control in pinacol formation, highlighting the potential of electrochemical synthesis as a superior alternative to traditional methods. By employing green electrodes, this work marks a significant advancement toward cleaner chemistry, opening new perspectives for the development of more efficient, sustainable, and environmentally respectful synthetic pathways.

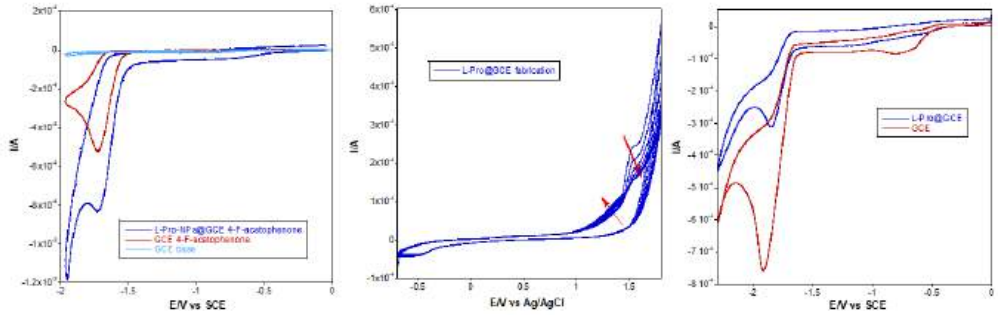

Fig. 1. *Left:* Voltammetry of the ketone with the L-Pro-NPs functionalized GC electrode (in blue). *Right:* Voltammetry of the ketone with the L-Pro functionalized GC electrode (in blue). *Center:* The 10 cycles of L-Pro functionalization.

	Cathode	Solvent	H_2O	Additive	I or E	F/mol	Pinacol (dl/meso)	dl-Pinacol e.r.
1	L-Pro-NPs@GC	CH_3CN	140 eq.	-	-1.7 V	2.5	82% (83/17)	Rac.
2	L-His@GC	CH_3CN	140 eq.	-	-1.85V	1.5	52% (84/16)	51/49
3	L-Ala-L-His@GC	CH_3CN	-	-	-2.20V	1.5	83% (74/26)	51/49
4	GC	DMSO	210 eq.	L-Phe 1 eq.	2 mA	3.0	93% (77/23)	Rac.

Table 1. Cathodic reduction of 4-fluoroacetophenone to the corresponding pinacol

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CCS - D3 - P05

Quantifying structural and dipole–dipole coupling effects in coverage-dependent CO infrared spectra on Pt

Xiang Yu[1], Nikolay Kosinov[2], Matteo Monai[1]

[1]Institute for Sustainable and Circular Chemistry, Utrecht University, Netherlands; [2]Inorganic Materials and Catalysis, Eindhoven University of Technology, Netherlands

Infrared (IR) absorption bands of adsorbates on catalyst surfaces are widely observed to shift as a function of surface coverage. Such coverage-dependent shifts may originate from two distinct physical mechanisms: adsorption-induced structural deformation of the active site, which modifies the local electronic environment, and dynamic dipole–dipole coupling (DDDC) between neighboring adsorbates, which alters vibrational frequencies without requiring structural reconstruction.

Using CO adsorption on Pt surfaces as a model system, we quantitatively assess both effects. Coverage-induced structural changes of Pt active sites and their impact on CO vibrational frequencies are evaluated using first-principles density functional theory (DFT) calculations combined with machine-learning-based predictions[1]. In parallel, the contribution from dynamic dipole–dipole coupling is investigated by implementing and programmatically extending the semi-empirical model proposed by Brandt[2], enabling quantitative simulations of vibrational coupling as a function of CO coverage, spatial distribution, and nanoparticle morphology.

The relative importance of structural and vibrational coupling effects on coverage-dependent CO frequency shifts is systematically evaluated and compared. Mixed $^{12}CO/^{13}CO$ isotopic adsorption is employed as a probe, both experimentally and theoretically, to disentangle the distinct physical origins of these two mechanisms[3]. This work provides a unified framework for interpreting coverage-dependent infrared spectra of adsorbates on metal catalysts and clarifies the respective roles of structural and vibrational interactions in CO infrared spectroscopy on Pt.

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CCS - D3 - P06

Addition polymerization of norbornene by Cobalt(II) and Palladium(II) complexes ligated *by N, N'*-bidentate iminomethylpyridine derivatives

Hyosun Lee
Dept. of Chemistry, Kyungpook National University, Republic of Korea

The addition polymerization of cyclic olefins has been played as a key technology for synthesizing special polymers with high thermal stability and excellent optical properties. We have synthesized the Co(II) and Pd(II) complexes, namely, **$[L_nMCl_2]$** (M = Co and Pd, L_n = L_A–L_C) supported by iminomethylpyridine derived ligands, such as (E)-N^1,N^1-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine (L_A), (E)-3-methoxy-N-(quinolin-2-ylmethylene)propan-1-amine (L_B), (E)-N-(pyridin-2-ylmethylene)hexan-1-amine (L_C)[1,2]. All complexes were characterized by ^{1}H NMR, ^{13}C NMR, FT-IR and elemental analysis. The X-ray single crystal diffraction revealed that **$[L_ACoCl_2]$** were distorted tetrahedral geometry, while **$[L_BCoCl_2]$** were distorted trigonal bipyramidal geometry. In contrast, Pd(II) complexes, **$[L_BPdCl_2]$** and **$[L_CPdCl_2]$** have shown a distorted square planar geometry around metal center. These complexes were used for the polymerization of norbornene (NB) in the presence of cocatalyst modified methylaluminoxane (MMAO) to give polynorbornene (PNB) at 25°C with high conversion and sterospecific enriched PNB. Specifically, **$[L_ACoCl_2]$** was observed that effectively catalyzed the norbornene with more than 98% conversion and maintained a narrow molecular weight distribution (PDI = 1.13) at 25°C in the presence of MMAO.

This research was supported by the National Research Foundation of South Korea, funded by the Ministry of Education, Science, and Technology (MEST) (Grant No. RS-2023-NR076653 and RS-2025-25415722).

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CCS - D3 - P07

Synthesis and structural characterization of cobalt(II) and palladium(II) complexes bearing *N*-substituted iminomethylpyridine and aminomethylpyridine derivative: Application to ring opening polymerization of *rac*-lactide

Eun Yeong Kim, Hyosun Lee*
Dept. of Chemistry, Kyungpook National University, Republic of Korea

The increasing demand for sustainable polymer materials highlights the need for stereocontrolled metal catalysts for the ring opening polymerization (ROP) of rac-lactide, a renewable monomer used in the production of biodegradable poly(lactic acid) (PLA). To address this challenge, two furfurylamine-derived *N,N'*-donor ligands, (*E*)-1-(furan-2-yl)-*N*-(pyridin-2-ylmethylene)methanamine (L_A) and 1-(furan-2-yl)-*N*-(pyridin-2-ylmethyl)methanamine (L_B) were synthesized through a condensation/reduction sequence and coordinated to anhyrous [$CoCl_2$] and [$Pd(MeCN)_2Cl_2$] to afford a series of metal complexes **[L_nMCl_2]** (L_n = L_A and L_B; M = Co and Pd).

The ligands and resulting complexes were characterized using ^{1}H and ^{13}C NMR spectroscopy, elemental analysis, FT-IR spectroscopy, and single crystal X-ray diffraction (SCXRD). Preliminary structural results indicate the formation of well-defined metal–ligand architecture, specifically by SCXRD analysis is being refined to elucidate the coordination environments, the influence of ligand frameworks, and metal centers on complex structure.

Catalytic evaluation is being conducted following activation with LiO^tBu to generate *in situ* metal alkoxide species known to initiate ROP. ROP studies at 0 °C and 25 °C aim to assess initiation efficiency, monomer conversion, and stereoregularity. Preliminary results indicate that the ligand backbone plays a significant role in modulating polymerization behavior, likely through steric and electronic effects at the metal center.

By integrating ligand design, coordination chemistry, and catalytic performance, this study seeks to identify molecular factors that promote efficient and selective lactide polymerization. The findings are expected to contribute to the rational development of sustainable transition metal-based catalysts for biodegradable PLA production and to inform future catalyst design in polymer chemistry.

This research was supported by the National Research Foundation of South Korea, funded by the Ministry of Education, Science, and Technology (MEST) (Grant No. RS-2023-NR076653 and RS-2025-25415722).

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CCS - D3 - P08
Chiral CN-palladacycles as precatalysts for alkoxycarbonylation of styrene derivatives

Vera Barrutia Fernando A.[1] , Amézquita Valencia Manuel[1]*
[1]Dept. of Inorganic Chemistry, Instituto de Química, Universidad Nacional Autónoma de México, México
** manuel.amezquita@iquimica.unam.mx*

Carbonylation reactions are powerful tools for the synthesis of carbonyl-containing compounds such as esters, amides, aldehydes, ketones, and acids, which are ubiquitous in pharmaceuticals and fine chemicals. Palladium-catalyzed alkoxycarbonylation of olefins provides an efficient route to ester derivatives; however, achieving high regio- and stereocontrol remains challenging. Palladacycles have emerged as robust and well-defined precatalysts due to their air and moisture stability and controlled ligand environments. While phosphine-stabilized CN-palladacycles are known to promote alkoxycarbonylation with high regioselectivity, the development of chiral variants capable of inducing asymmetry is still largely unexplored.
Herein, we report the synthesis of chiral CN-palladacycles obtained via ortho-palladation of chiral imines and their preliminary evaluation in alkoxycarbonylation reactions using alcohols as nucleophiles under acidic CO conditions. The chiral palladacycles were obtained in moderate to good yields (typically >80%) and displayed high stability toward air and moisture. Their structures were confirmed by multinuclear NMR spectroscopy, IR spectroscopy, and mass spectrometry.
Preliminary catalytic studies in the alkoxycarbonylation of styrene derivatives revealed that a representative chiral complex achieved a conversion of approximately 67% while maintaining a pronounced regioselectivity toward the branched ester product (B:L ≈ 90:10). Importantly, the introduction of chiral substituents on the imine fragment did not compromise catalytic activity or regioselectivity, indicating that the chiral environment is well accommodated within the catalytic framework. These results represent an initial step toward the development of asymmetric alkoxycarbonylation processes based on chiral CN-palladacycle precatalysts. Ongoing work is focused on expanding the substrate scope and further optimization to evaluate potential asymmetric induction.

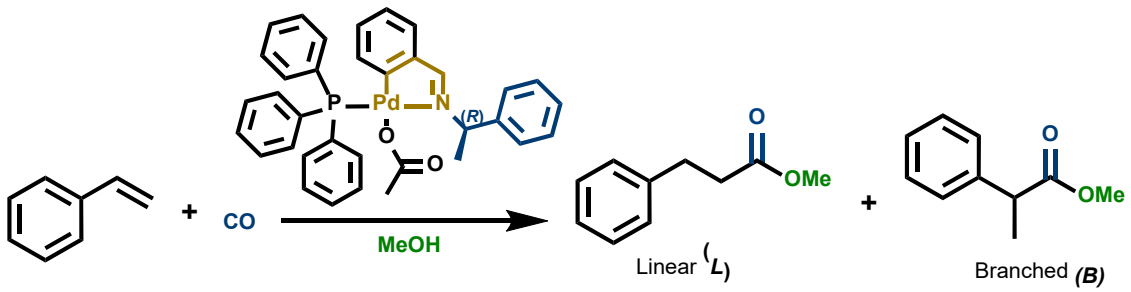

Fig. 1. Representative alkoxycarbonylation of styrene catalyzed by a chiral CN-palladacycle.
*Reaction conditions: Styrene (0.34 mmol), Pd complex (1 mol%), MsOH (5 mol%), LiCl (8 mol%), 5 mL of CH2Cl2: ROH (4:1, v/v), CO (400 psi), 80 °C, 12 h.

Acknowledgments: The authors gratefully acknowledge the financial support from Universidad Nacional Autónoma de México (UNAM) and the Instituto de Química. We also thank the technical staff of the Dept. of Inorganic Chemistry for analytical and instrumental support.

CCS - D3 - P09

Enhanced photocatalytic degradation of phenols using g-C_3N_4-supported phthalocyanine catalysts

Cagla Akkol[1*],Ece Tugba Saka[1]
[1]Karadeniz Tech Univ, Fac Sci, Dept Chem, Trabzon, Turkiye
akkolcagla@gmail.com

Phenolic compounds are widely recognized as persistent organic pollutants frequently detected in industrial wastewater, posing serious environmental and human health risks [1]. In this study, novel phthalocyanine-based photocatalysts supported on graphitic carbon nitride (g-C_3N_4) were developed to enhance the photocatalytic degradation of phenols under visible-light irradiation. The catalysts were synthesized via a rational molecular design strategy employing bio-derived aromatic precursors, with the aim of improving light-harvesting capability and charge transfer efficiency.

The successful synthesis and structural integrity of the g-C_3N_4-supported phthalocyanine catalysts were confirmed using various spectroscopic and physicochemical characterization techniques [2]. Photocatalytic performance was systematically evaluated through the degradation of phenol in aqueous media, and the effects of key operational parameters—including irradiation time, catalyst dosage, and initial phenol concentration—were thoroughly investigated [3].

The hybrid photocatalysts exhibited significantly enhanced photocatalytic activity compared to unsupported phthalocyanine systems. This improvement is attributed to superior visible-light absorption, efficient charge separation, and accelerated interfacial electron transfer facilitated by the g-C_3N_4 support. Furthermore, the results indicate that both the molecular structure of the phthalocyanine and the nature of the central metal ion play critical roles in determining photocatalytic efficiency [4].

Overall, this study demonstrates that g-C_3N_4-supported phthalocyanine photocatalysts represent a promising and sustainable approach for the efficient removal of phenolic pollutants from water.

This study was supported by The Research Fund of Karadeniz Technical University (Project no: 16562).

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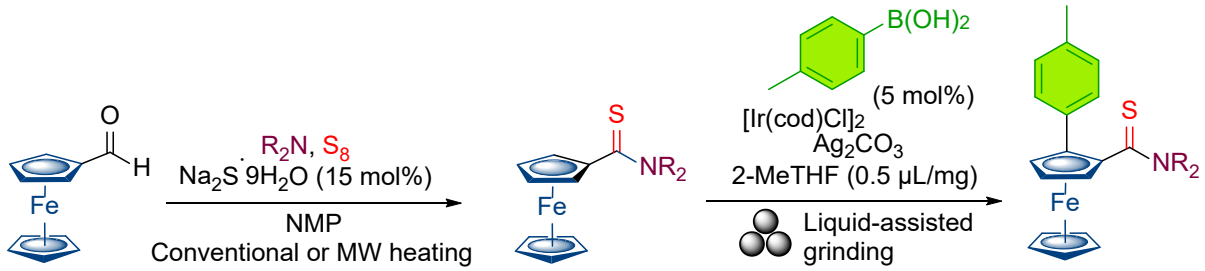
CCS - D3 – P10
Preparation of ferrocene thioamides and their mechanochemical C-H arylation

Henrich Kabzan[1], Péter Kisszékelyi[1], Juraj Filo[1], Marek Cigáň[1], Erik Rakovský[2], Radovan Šebesta[1]
[1]Dept. of Organic Chemistry, Comenius University Bratislava, Slovakia; [2]Dept. of Inorganic Chemistry, Comenius University Bratislava, Slovakia

A diverse series of ferrocene thioamides was obtained by the multicomponent Willgerodt-Kindler reaction of ferrocenecarboxaldehyde with various primary or secondary amines and sulfur in the presence of $Na_2S{\cdot}9H_2O$ (Scheme 1). Comprehensive solvent screening shows that amide-type solvents greatly enhance the reaction. On the other hand, this reaction is constrained by the steric hindrance of the bulky amine substrates. While conventional heating is sufficient for secondary amines, primary amines give better results under microwave irradiation at elevated temperature. Investigation of the reaction mechanism by NMR kinetic measurements as well as UV-Vis spectroscopy revealed that sodium sulfide serves as a promoter and not as a catalyst.[1] Selected ferrocene thioamides were subsequently used as substrates for the study of mechanochemical C-H arylations. C-H activations represent modern methods of organic synthesis, which are currently receiving great attention due to their economic and environmental benefits. A major disadvantage of many C-H activation reactions is their long reaction times, often ranging from 12 to 24 hours. This limitation can be overcome by mechanical grinding in a ball mill, which often accelerates the reaction and improves the product yields. Mechanochemical Ir-catalyzed C-H arylation of ferrocene thioamides using *p*-tolylboronic acid as an aryl source and Ag_2CO_3 as an oxidizing agent furnishes a range of *ortho*-arylated thioamides (Scheme 1). Among the LAG additives tested, 2-MeTHF proved to be the most suitable option. The reaction requires heating the milling jar to a temperature of 60 °C. For this purpose, a heating bandage connected to a thermostat is used.



Scheme 1. Synthesis of ferrocene thioamides followed by mechanochemical C-H arylation.

This work was supported by the Slovak Grant Agency VEGA, grant no. 1/0464/25.

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CCS - D3 – P11

Iron-porphyrin catalyzed deaminative hydrobenzylation of alkenes using redox-active pyridinium salts

Kevin Bucher[1], Julien Doulcet[2]
[1]Lancaster University, UK; [2]Lancaster University, UK

All-carbon quaternary centres are highly valued motifs in drug discovery, as increasing the fraction of sp^3 carbons correlates with improved clinical success[1]. These centres impart conformational rigidity and molecular complexity, enhancing aqueous solubility, metabolic stability, and selective protein binding through their three-dimensionality relative to sp^2-rich scaffolds[2]. Although prevalent in natural products and natural product-derived drugs[3], quaternary carbons remain synthetically challenging to access using traditional two-electron polar disconnections, which often require harsh conditions and multistep sequences that limit efficiency and functional group tolerance.

Radical cross-coupling strategies have begun to address these challenges. MacMillan's S_H2 platform enabled selective coupling of primary and tertiary carbon-centred radicals under mild conditions using an iron–porphyrin catalyst[4]. Subsequent incorporation of metal-hydride hydrogen atom transfer (MHAT) catalysis by Baran and Shenvi[5] allowed direct generation of tertiary radicals from alkenes. Coupling with diverse primary radical precursors — including redox-active esters, benzyl bromides, 1,4-dihydropyridines, and alcohols[5–8] — has provided new approaches to $C(sp^3)$–$C(sp^3)$ quaternary carbon formation.

Here, we report a deaminative hydrobenzylation strategy that merges MHAT with a reductive pathway using N-benzylpyridinium salts and a commercially available iron–porphyrin catalyst. This approach simplifies precursor preparation and avoids specialized catalysts. The method enables efficient $C(sp^3)$–$C(sp^3)$ bond formation between alkenes and benzylic amines across 45 examples, delivering 25–92% isolated yields. Mechanistic studies, including radical probes and spectroscopic analysis, support a radical-intermediate pathway involving EDA complex formation.

The operational simplicity, broad scope, and mechanistic insight of this platform highlight its utility for late-stage functionalisation and rapid construction of densely substituted, drug-relevant scaffolds.

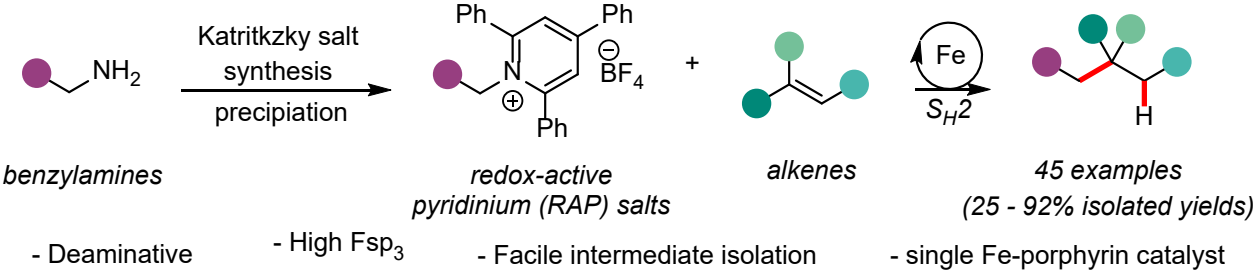

Fig. 1. Deaminative hydrobenzylation of alkenes via MHAT/S_H2 catalysis. Benzylic amines are converted to redox-active N-benzylpyridinium salts, which undergo iron–porphyrin-catalyzed radical cross-coupling with alkenes to furnish all-carbon quaternary centers.

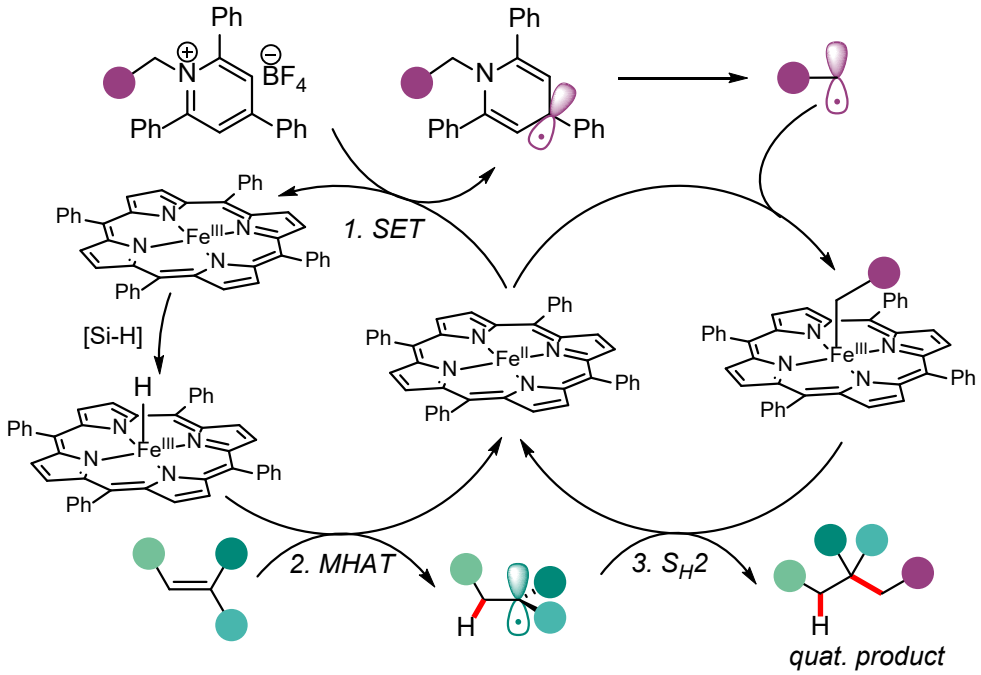

Fig. 2. Proposed mechanism showing SET activation of the pyridinium salt, MHAT generation of a tertiary radical, and S_H2 cross-coupling to form the quaternary carbon product.

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CCS - D3 – P12
Understanding and tuning the reduction of nitro-compounds in water at carbon surfaces

Aoyang Liu, Maya Landis, Michail Stamatakis, Kylie A. Vincent
University of Oxford, Dept. of Chemistry, UK
aoyang.liu@jesus.ox.ac.uk

Amine compounds play a crucial role in pharmaceutical chemistry and many areas of the chemical industry, as they are key structural motifs in a wide range of biologically active molecules and functional materials. Therefore, understanding the synthesis of amine group is essential. Both aliphatic and aromatic nitro compounds are reduced readily at carbon electrodes in aqueous electrolyte. Reduction of nitroarenes typically gives the amine (aniline) product, via a hydroxylamine intermediate. This has been exploited in hydrogenation (bio)catalysts that use a H_2-activating site (e.g. the hydrogenase enzyme) to supply electrons to the carbon surface, so that nitro compounds can be reduced at the carbon.[1] A similar mechanism can occur with Pd/C catalysts, where Pd catalyzes H_2 oxidation, and the carbon is responsible for nitro-group reductions.[2] Although the carbon is typically considered just a *support*, it actually appears to have an electrocatalytic role, since different carbon materials can tune the onset potential for nitro reduction. This project explores electrocatalytic reduction of model nitro compounds, nitrobenzene, nitrophenol and nitrohexane, at different carbon surfaces to evaluate onset potential, and selectivity for hydroxylamine to amine. This will pave the way for a computational study to evaluate interactions of nitro compounds with the carbon materials and the mechanism for their reduction. This poster presents electrochemical analysis and preliminary plans for the computational work.

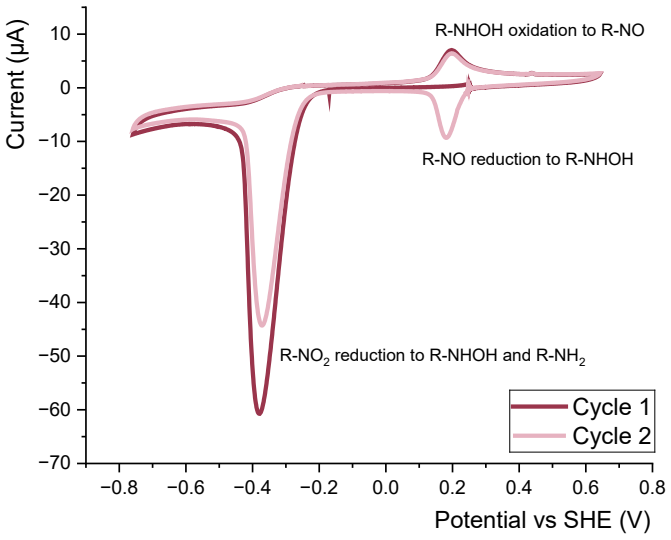

Fig. 1. Cyclic voltammogram of 1 mM nitrobenzene in sodium phosphate buffer (50 mM, pH=6.0) at a pyrolytic graphite 'edge' working electrode, scan rate 10 mV/s at 25℃.

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CCS - D3 – P13
Utilization Of 2D transition-metal dichalcogenide supports for rhodium-catalyzed hydroformylation

Martina Pitínová[1], Alica Krnáčová[1], Ayesha Shafiq[1], Jáchym Kučera[1], Iryna Danylo[1], Lukáš Koláčný[1], Martin Veselý[1]*
[1]Dept. of Organic Technology, University of Chemistry and Technology Prague, Czech Republic

Two-dimensional transition-metal dichalcogenides (TMDs) have recently attracted increasing attention as catalyst supports due to their layered structure, tunable electronic properties, and strong metal–support interactions enabling stabilization of highly dispersed active species. In this work, we investigate the utilization of MoS_2 [1]and WS_2 [2]as supports for rhodium-based heterogeneous catalysts for styrene hydroformylation, aiming to develop recyclable catalytic systems with performance approaching that of homogeneous rhodium complexes.
Rhodium catalysts with loadings between 0.5 and 10 wt.% were prepared by wet impregnation under different temperatures, followed by optional thermal treatments. The influence of preparation conditions on catalyst structure and performance was studied using XRF, XRD, N_2 physisorption, SEM, TEM, and temperature-programmed desorption of pyridine. Both MoS_2- and WS_2-based catalysts showed formation of highly dispersed Rh nanoparticles with typical sizes below 5 nm, located on the surface of layered sulphide supports. The layered morphology together with the presence of sulphur vacancies enables strong anchoring of Rh species and provides an electronic environment that can influence key steps of the hydroformylation mechanism.
Catalytic testing in styrene hydroformylation (CO/H_2, 3 MPa, 100 °C) revealed that both supports allow achieving high aldehyde selectivity around 80 %, comparable to the homogeneous Wilkinson catalyst, while preserving the advantages of heterogeneous systems such as easy separation and potential reuse. Optimal performance was obtained for catalysts with Rh loading ≥ 2 wt.% prepared under mild conditions. In contrast, high-temperature calcination led to partial sulphur loss, formation of oxide phases, increased surface acidity, and a higher tendency toward oligomerization and hydrogenation side reactions, resulting in decreased aldehyde selectivity.
The results demonstrate that layered TMD materials act as ligand-like supports that stabilize catalytically active Rh species and confirm that 2D supports represent a promising platform for designing selective heterogeneous hydroformylation catalysts.

This research was supported by the Czech Science Foundation (GACR No. 23–08083M) and by the institutional support Dagmar Procházková Fund provided by University of Chemistry and Technology in Prague.

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CCS - D3 – P14

Atroposelective access to oxicam-inspired axially chiral benzopyrano[1,2]thiazinone S,S-dioxides via oxidative NHC catalysis

Monika Radosińska[1], Zbigniew Rafiński[1]
[1]Faculty of Chemistry, Chair of Organic Chemistry, Nicolaus Copernicus University in Toruń, Poland
**Corresponding author: m.radosinska@doktorant.umk.pl*

Atropisomerism, a stereochemical phenomenon arising from restricted rotation around σ bonds, can afford configurationally stable axially chiral molecules. Owing to their importance in asymmetric catalysis, drug discovery, and functional materials, the development of efficient atroposelective synthetic strategies remains a significant challenge. In particular, the catalytic construction of a stereogenic C–C axis within densely functionalized and polycyclic systems requires precise control over both reactivity and conformational stability[1]. In this context, N-heterocyclic carbenes (NHCs) have emerged as powerful organocatalysts, enabling diverse transformations through both umpolung and non-umpolung reactivity modes. Their unique ability to generate reactive intermediates under mild conditions, combined with tunable steric and electronic properties, allows for precise control – yet their application in constructing axially chiral benzothiazine-based scaffolds has remained unexplored[1,2].

Herein, we present an atropoenantioselective oxidative NHC-catalyzed approach to benzopyrano[1,2]thiazinone S,S-dioxides bearing a stereogenic C–C axis. The strategy is based on an oxicam-inspired benzothiazine 1,1-dioxide core, a scaffold structurally related to the oxicam class of nonsteroidal anti-inflammatory drugs (NSAISs)[3,4]. By introducing axial chirality into this framework, we expand beyond conventional point-chiral oxicam-derived systems and access structurally complex polycyclic architectures. The developed methodology provides products with high enantioselectivity (up to 92% ee), demonstrating effective stereocontrol under oxidative NHC catalysis.

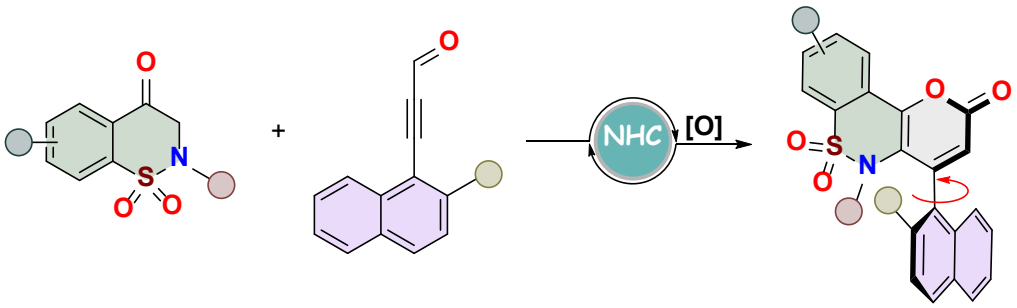

Fig. 1. NHC-catalyzed synthesis of tricyclic α-pyranones with chiral C–C axis.

Project co-financed by the National Science Center within the framework of the program PRELUDIUM BiS 4 (UMO – 2022/47/O/ST4/02432).

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CCS - D3 – P19

Novel Bi_3O_4Br/TiO_2NB/glucose hydrochar for photocatalytic degradation of pharmaceuticals

Sajad Ahmadi[1], Velma Beri Kimbi Yaah[2], Sergio Botelho de Oliveira[3], Satu Ojala[1]

[1]Environmental and Chemical Engineering unit, Faculty of technology, University of Oulu, Finland; [2]Nano and Molecular Systems Research unit, Faculty of Science, University of Oulu, Finland; [3]Dept. of Chemistry, Federal Institute of Goiás, Brazil

To harness their synergistic effects, novel ternary composite photocatalysts containing Bi_3O_4Br, TiO_2 nanobelts, and glucose hydrochar were developed using one step and two steps hydrothermal synthesis for the visible-light degradation of pharmaceuticals. Hydrochar, despite its lower energy requirement, defect-rich structure, abundant oxygen-containing functional groups and effective role as an electron shuttle that could enhance charge transfer, it has remained underexplored compared to the biochar component (1-2). Hence in this work, we explored the unique importance of the one-step versus two-step hydrothermal synthesis. Different ratios (5, 10, 15, and 20%) of the glucose hydrochar was used to synthesize the Bi_3O_4Br/TiO_2NB/GH photocatalysts. In the one-step hydrothermal method, glucose, TiO_2NB, and Bi_3O_4Br precursors were combined and hydrothermally treated simultaneously, whereas in the two-step hydrothermal method, glucose hydrochar was first formed on TiO_2NB, followed by a second hydrothermal step to grow Bi_3O_4Br on the pre-formed TiO_2NB/GH composite. Extensive characterization of the prepared materials revealed that, the two-step method promoted Bi_3O_4Br nanosheet growth on hydrochar. Overall, the incorporation of hydrochar into the Bi_3O_4Br/TiO_2NB photocatalyst primarily enhanced interfacial electronic coupling and charge-transfer efficiency (Fig.1). DRIFT spectroscopy revealed abundant oxygen-containing functional groups on hydrochar, which facilitate interfacial interactions and electron shuttling. These interactions were directly confirmed by XPS through consistent negative shifts in Ti 2p, Bi 4f, Br 3d, and O 1s binding energies, evidencing strong electronic coupling. UV-Vis DRS showed enhanced visible-light absorption without significant bandgap alteration, attributed to hydrochar's light-harvesting capability The two-step 10% photocatalyst achieved the highest degradation efficiency (91%) at natural pH under visible LED irradiation. Scavenger tests (Fig.2) and EPR identified the dominant reactive species, while selective Pt and MnO_x photodeposition confirmed a Z-scheme mechanism with hydrochar acting as an effective electron mediator. The photocatalyst also exhibited potential for treating real pharmaceutical wastewater.

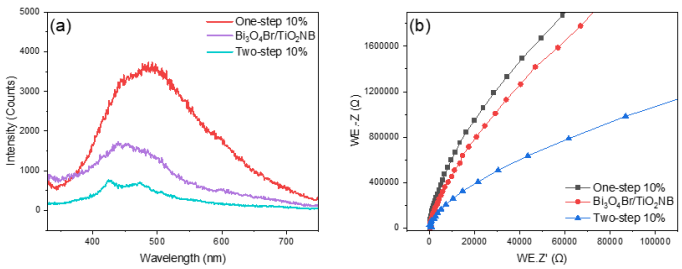

Fig. 1. (a) Photoluminescence and (b) Electrochemical impedance analysis

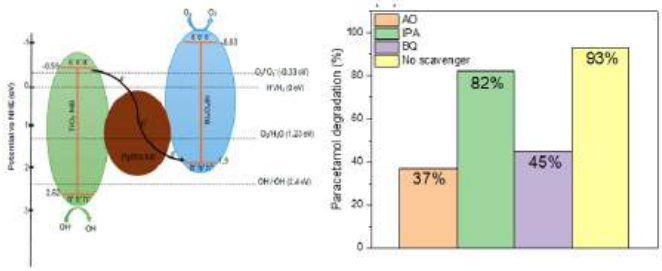

Fig. 2. Proposed mechanism and scavenger analysis

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CCS - D3 – P20

V_2O_5/CeO_2 catalyst for selective oxidative C-N coupling of amines and alcohols into imines

Nagendra Kulal[1], Bassam Elali[1,2] and Sani Abdullahi Zarewa[2]

[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Chemistry Dept., King Fahd University of Petroleum and Minerals, Saudi Arabia

The oxidative coupling of alcohols and amines to produce imines, commonly known as Schiff bases, is an important transformation in the synthesis of fine chemicals, dyes, insecticides, and pharmaceuticals. Traditional methods often rely on noble metal catalysts, which are expensive, less sustainable, and encounter difficulties in catalyst recovery and reusability. CeO_2 is an alternative and promising support due to its unique redox properties and high density of oxygen vacancies that facilities the oxidative C-N coupling of amine and alcohol. In the work V_2O_5/CeO_2 catalysts were studied to enhance its catalytic activity. The synthesized catalysts were systematically characterized and correlated with its catalytic performance. Among the catalysts screened, the V_2O_5/CeO_2 catalyst exhibits 97.0 of benzyl alcohol conversion and 100.0% of selectivity for N-benzylideneaniline. Further, the N-benzylideneaniline product was purified and isolated by column and thin-layer chromatography.

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CCS - D3 – P21

A sustainable MgO@EDTA@Ag nanocatalyst for eco-friendly xanthene formation and efficient rhodamine B degradation

Anamika Brahma[1], Snigdha Singh*[1,2]
[1]Dept. of Chemistry, University of Delhi, India; [2]Institute for Nanomedical Sciences (INMS), University of Delhi, India

The development of environmentally benign and high-performance catalytic systems is essential for advancing green chemistry and effective environmental remediation. In this study, a MgO@EDTA@Ag nanocomposite was successfully synthesised and employed as a multifunctional heterogeneous catalyst for the sustainable synthesis of xanthene derivatives and the efficient degradation of Rhodamine B dye. The presence of EDTA provided strong surface coordination sites, facilitating effective anchoring of silver nanoparticles and enhancing electron transfer processes and reactive species generation, which are crucial for catalytic activity. The synthesised nanocatalyst was comprehensively characterised using XRD, XPS, FESEM, TEM, FTIR, EDAX, TGA, nitrogen adsorption-desorption studies, and BET analysis. These techniques confirmed the successful formation of the nanocomposite, along with its structural stability, favourable surface morphology, high thermal stability, and large specific surface area. The MgO@EDTA@Ag nanocatalyst exhibited excellent catalytic performance, as supported by favourable green chemistry metrics, including a low E-factor (0.23), a low process mass intensity (PMI=1.23), a high reaction mass efficiency (RME=90.06%), and a high carbon efficiency (CE=90%). Additionally, the catalyst demonstrated good recyclability and environmental compatibility, highlighting its suitability for sustainable chemical synthesis and wastewater treatment applications. Notably, in photocatalytic degradation studies, the catalyst achieved 96% degradation of Rhodamine B within 60 minutes using only 0.02 mg of catalyst in 2 mL of dye solution, demonstrating its high efficiency and potential for practical environmental remediation.

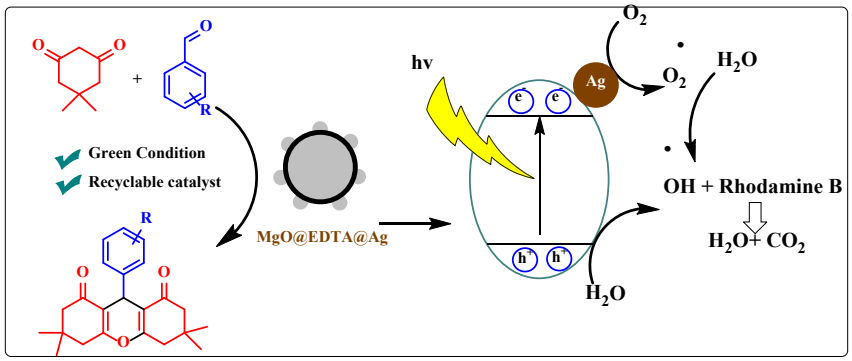

Fig. 1. Graphical abstract

S.S. and A. Brahma acknowledge the Dept. of Chemistry and the Institute for Nanomedical Sciences (INMS), University of Delhi, for infrastructural support, and USIC for instrumental facilities. A. Brahma (Grant No. 231610191350) gratefully acknowledges UGC-JRF for financial assistance.

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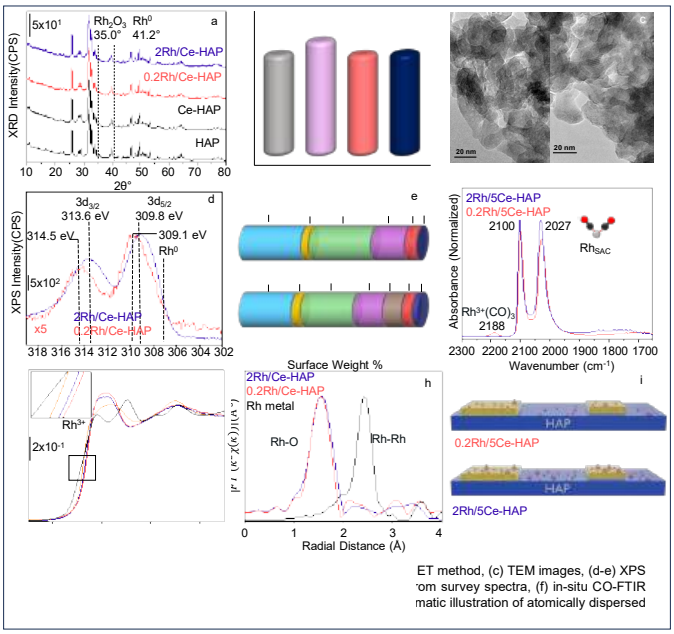
CCS - D3 – P23

From isolated Rh single atom catalytic sites to cooperative single atom ensembles: Tuning catalytic pathways in CO_2 and ethanol interactions

Ayse Dilay Erdali[1], Yusuf Kocak[1], Kaan Karaca[1], Messaoud Harfouche[2], Ahsan Jalal[1], Ahmet Kerim Avcı[3], and Emrah Ozensoy[1,4*]

[1]Dept. of Chemistry, Bilkent University, Ankara, Türkiye; [2]Synchrotron-Light for Experimental Science and Applications in the Middle East (SESAME), Allan, Jordan; [3]Dept. of Chemical Engineering, Bogazici University, Bebek, Istanbul, Türkiye; [4]UNAM-National Nanotechnology Center, Bilkent University, Ankara, Türkiye

**Corresponding author: ozensoy@fen.bilkent.edu.tr*



ET method, (c) TEM images, (d-e) XPS om survey spectra, (f) in-situ CO-FTIR matic illustration of atomically dispersed

Co-adsorption of ethanol and CO_2 on Rh single-atom catalysts (SACs) with different metal loadings (0.2 wt% and 2 wt% Rh) supported on ceria-promoted hydroxyapatite (Ce-HAP) in relevance to ethanol dry reforming reaction ($C_2H_5OH(g) + CO_2(g) \rightarrow 3CO(g) + 3H_2(g)$) was investigated via multimodal spectroscopic, imaging and diffraction techniques (i.e., in-situ FTIR, TPD, XANES, EXAFS, XPS, TEM, and XRD). Upon ethanol and CO_2 adsorption at 50 °C, Rh^{3+} species on 0.2Rh/Ce-HAP led to the formation of ethoxides, carbonates, and bicarbonates. Increasing the temperature to 350 °C resulted in oxidation of adsorbed ethoxide species to acetate. In contrast, 2Rh/Ce-HAP catalyst exhibited relatively reduced $Rh^{(3-x)+}$ and $Ce^{(4-y)+}$ sites as opposed to 0.2Rh/Ce-HAP, where 2Rh/Ce-HAP facilitated ethoxide decomposition to acetaldehyde, CO, and CH_4 via C-C/C-H bond activation. This behavior suggested a noticeable difference in the reactivity patterns where a catalytic route including ethoxide oxidation to acetate is replaced with an alternative route comprised of ethoxide dehydrogenation and C-C/C-H bond scission with increasing Rh loading. Our results indicate that while reactivity of SACs at low loadings may be predominantly dictated by isolated single Rh sites, at extremely high loadings, cooperative action of multiple Rh SAC sites located in proximity of Rh clusters which are generated in-situ can lead to significant differences in catalytic reaction mechanisms. Accordingly, the current findings provide valuable molecular-level insights into the design of novel SAC catalysts with varying catalytic selectivity and reactivity as a function of platinum-group-metal (PGM) loading.

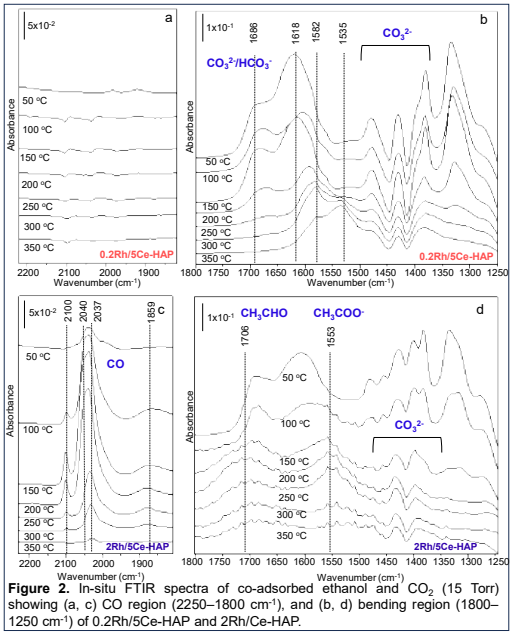


Figure 2. In-situ FTIR spectra of co-adsorbed ethanol and CO_2 (15 Torr) showing (a, c) CO region (2250–1800 cm^{-1}), and (b, d) bending region (1800–1250 cm^{-1}) of 0.2Rh/5Ce-HAP and 2Rh/Ce-HAP.

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CCS - D3 – P25

New N-heterocyclic carbene platinum complexes – synthesis, characterisation and catalytic activity.

Anna Smoczyńska[1], Sylwia Ostrowska[1], Steven P. Nolan[2] Cezary Pietraszuk[1]

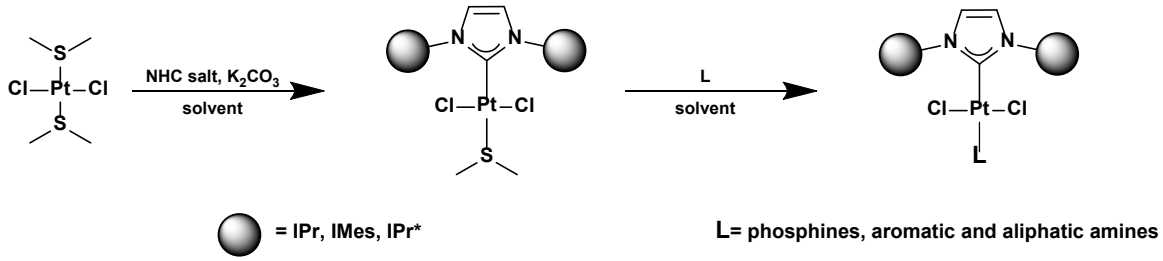
[1]Adam Mickiewicz University, Faculty of Chemistry, Poland; [2]Dept. of Chemistry and Center for Sustainable Chemistry, Ghent University, Belgium

Platinum complexes have attracted considerable interest for many years due to their unique properties and applications in catalysis.[1]

In particular, platinum complexes bearing N-heterocyclic carbene (NHC) ligands exhibit notable catalytic activity in processes such as hydrometallation, dimetallation, hydroamination.[2] Appropriate ligand design can not only enhance the catalytic efficiency of platinum but also enable precise control over reaction selectivity.

This work focuses on the synthesis, characterization, and investigation of the catalytic activity of the N-heterocyclic carbene platinum complexes. In particular, the aim of the syntheses was to obtain complexes with sterically bulky carbene ligands.

The synthesis is based on an approach consistent with the principles of green chemistry, leading to the formation of the [$PtCl_2$(NHC)(DMS)] complex[3], followed by a ligand substitution step in which the DMS ligand is replaced by another ligand.



Drawing 1 General synthesis of platinum complexes[3]

The synthesized complexes were characterized using spectroscopic techniques as well as single-crystal X-ray diffraction analysis. The resulting complexes are applied in catalysis and are also investigated for their potential biological properties. Their catalytic performance was evaluated in Suzuki[4] and selected other coupling reactions.

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CCS - D4 - P04

Modification of Ni/Al_2O_3 catalysts by incorporating graphitic Carbon Quantum Dots (CQDs) for selective CO_2 hydrogenation to CO

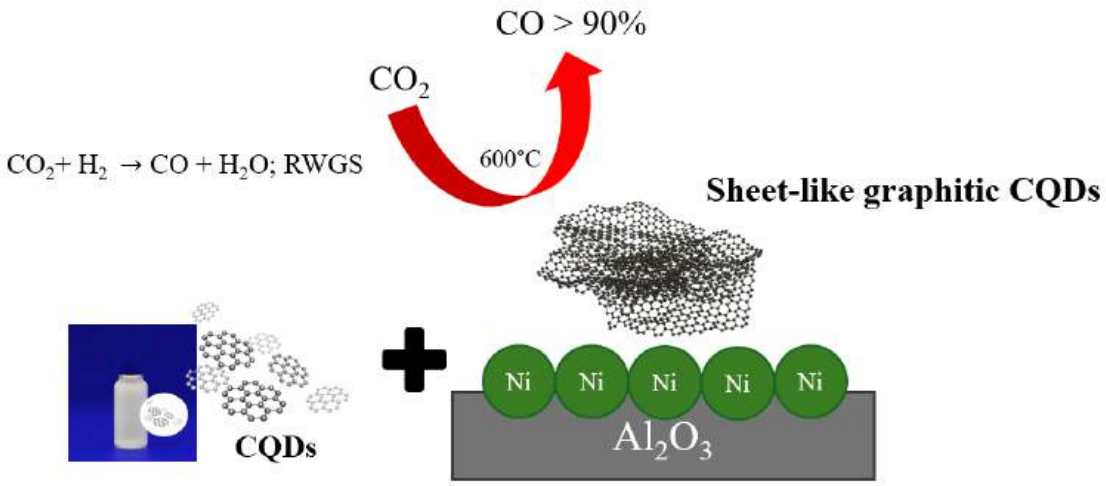
Supichcha Sukserm[1], Suthasinee Watmanee[2], Joongjai panpranot[1], Weerachon Tolek[1], Francisco J. Cadete Santos Aires[3], Eric Ehret[3]

[1]Dept. of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Thailand; [2]Dept. of Chemical Engineering, Faculty of Engineering, Kasetsart University, Thailand; [3]Institut de Recherches sur la Catalyse et l'Environnement de Lyon, France

CO_2 emissions are a major driver of global warming and climate change. One promising mitigation strategy is the hydrogenation of CO_2 into fuels and chemicals. However, despite CO being a crucial intermediate for producing higher-value liquid hydrocarbons and oxygenates, achieving high CO selectivity over Ni catalysts remains challenging. In this study, 15 wt.% Ni/Al_2O_3 catalysts (15Ni) were modified with 3 wt.% graphitic carbon quantum dots (CQDs) via incipient impregnation and calcination under N_2 at 600 °C for 5 h. The structural and surface properties were characterized by SEM-EDX, TEM-EDX, ETEM, XRD, XPS, ICP, TGA, TPO-MS and H_2-TPR-MS analyses.

While the convetional 15Ni catalyst mainly yielded methane and formed soft coke after 10 h at 600°C, the incorporation of CQDs markedly enhanced CO selectivity. The 15Ni3CQD catalyst achieved ~90% CO selectivity with ~57% CO_2 conversion, with no evidence of soft coke formation. Moreover, CQDs underwent in situ transformation into sheet-like graphitic carbon layers on the catalyst surface, contributing additional value. These findings demonstrate that CQDs promote the reverse water–gas shift (RWGS) pathway while suppressing methanation, thereby steering Ni-based catalysts toward CO production. Overall, this work highlights CQDs as an effective, scalable, and non-noble modifier for CO_2 hydrogenation, offering a promising route for sustainable CO_2 utilization.

Graphical abstract:



CCS - D4 - P07
Sustainable synthesis of 2,4,6-trisubstituted pyridines using surface-modified PET@UiO-66 vials

Yogendra Kumar and Subbiah Nagarajan*
National Institute of Technology Warangal, India

This study demonstrates the modification of a polyethylene terephthalate (PET) surface to fabricate a metal-organic framework (MOF)-based UiO-66 vial for application in multicomponent reactions.[1] We report the development of a PET@UiO-66 vial that functions as an efficient, robust, and reusable heterogeneous catalyst for the sustainable synthesis of 2,4,6-trisubstituted pyridines via a multicomponent reaction strategy.[2] The structural and morphological features of the fabricated PET@UiO-66 vial were systematically characterized using powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR), optical microscopy, and field-emission scanning electron microscopy (FESEM). Nitrogen adsorption-desorption isotherm analysis revealed a specific surface area of 564.36 m^2g^{-1}, a maximum pore volume of 0.06 cm^3g^{-1}, and an average pore diameter of 3.05 nm.[3] Optimization of the reaction parameters indicated that the use of tert-butyl hydroperoxide (TBHP) as an oxidant in tetrahydrofuran (THF) at 60 °C afforded good to excellent yields of the desired products. The key advantages of this methodology include the high stability of the surface-modified vials, excellent recyclability, and operational simplicity, making it a sustainable and practical approach for heterocycle synthesis.

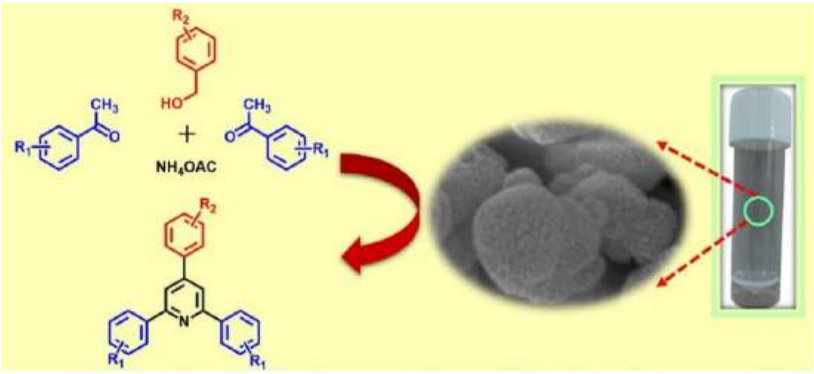


Fig. 1. Fabrication of a reusable PET@UiO-66 vessel for sustainable multicomponent synthesis of trisubstituted pyridines.

We greatly acknowledge the financial support from the SERB (sanction order no: CRG/2023/002466) and DST FIST (SR/FST/CS-II/2018/65). The authors gratefully acknowledge the University Grants Commission (UGC) for the research fellowship and the National Institute of Technology Warangal for providing infrastructural support.

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CCS - D4 - P18

Bubbles templated porous CeSe2/Co3Se4 heterostructures supported on Ni foam for CO2-free selective methanol oxidation to enhance green hydrogen production

Farhan Arshad[1], Mohammed A. Gonda[1,2*], Mohamed Jaffer Sadiq Mohamed[2], Munirah A. Almessiere[3,4]
[1]Interdisciplinary Research Center for Hydrogen Technologies & Carbon Management, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Laser Research Group, Dept. of Physics, K. A. CARE Energy Research and Innovation Center, King Fahd University of Petroleum and Minerals, Saudi Arabia; [3]Dept. of Physics, College of Science, Imam Abdulrahman Bin Faisal University, Saudi Arabia; [4]Dept. of Biophysics, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University, Saudi Arabia

This study investigates methanol-assisted water splitting (MAWS) as a promising alternative to conventional water electrolysis, with a focus on developing novel electrocatalysts to enhance the efficiency and selectivity of the methanol oxidation reaction (MOR) and the hydrogen evolution reaction (HER). A three-step synthesis process (electrodeposition, annealing, and selenization) was employed to synthesize the bubble-templated porous CeSe2/Co3Se4 heterostructures supported on nickel foam (CeCoSe@NF). The electrocatalyst's activity and selectivity for MOR to formate were tested, and its performance was evaluated by Operando electrochemical impedance spectroscopy (EIS) and H-NMR. The optimized electrocatalyst required a potential less than 1.35 V vs. RHE to initiate the methanol oxidation reaction, achieving a current density of 100 mA cm−2 at just 1.44 V vs. RHE under alkaline conditions. Operando EIS further confirms that MOR begins at 1.3 V for the porous CeCoSe@NF electrocatalyst, and MOR occurs similarly to OER at the low-frequency interface, indicating that MOR activity comes from the same adsorption intermediate (OH*) as OER. For overall methanol-assisted water electrolysis, the optimized porous heterostructured CeO2/Co3O4@NF electrode (CeCo@NF) without selenization showed good performance for HER, requiring 170 mV overpotential to attain 100 mA cm-2 current density with near 98 % Faradaic efficiency. The two-electrode integrated electrolyzer (CeCoSe@NF as the anode and CeCo@NF as the cathode), with methanol-assisted splitting, operates at a cell voltage of only 1.52 V to reach 20 mA cm-2, which is significantly lower than the 1.65 V required for traditional water splitting under the same conditions. The superior performance is attributed to the porous, dendritically interconnected nanostructure, synergistic heterointerfaces, and strong electronic coupling between the active components and the conductive Ni foam. This study highlights the potential of targeted methanol oxidation as a dual-purpose strategy for efficient energy-saving hydrogen generation and methanol upgrading to formate, contributing to the development of more sustainable energy systems.

CCS - D4 - P22

4,4'-oxybis-benzoic acid-based pristine MOFs as reusable, heterogeneous catalyst for hydrogenation reactions

Sreenidhi M Varma, Sundaram Ganesh Babu*
Nano-Catalysis Research Lab, Dept. of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, India

The large surface area, adjustable pore environment, and modular structural design of Metal-Organic Frameworks (MOFs) make MOFs a flexible class of porous crystalline materials with enormous potential in heterogeneous catalysis. The development of transition metal-based MOF catalytic systems for industrially significant organic transformations is the main goal of this effort; major focus on hydrogenation reactions, dehalogenation processes, and carbon–carbon and carbon–heteroatom coupling reactions. To modify active sites, electrical characteristics, and catalytic accessibility, several mono-metallic, bi-metallic, and bi-linker MOFs are created by carefully choosing metal nodes and organic linkers[1]. The integration of several 3d transition metals and mixed linkers is investigated to provide synergistic effects, improve catalytic efficiency, and expand substrate scope. The 3d transition metals such as Ni, Mn, Zn, and Cu-based MOFs are synthesized *via* the traditional solvothermal method using the organic linker 4,4'-oxybis-benzoic acid (OBA), which is a pristine linker with much enhanced coordination towards metals for the framework development. The structural integrity and characteristics of the produced MOFs are methodically assessed using spectroscopic techniques[2]. These MOFs demonstrate effective catalytic activity, selectivity, and recyclability under mild and sustained reaction conditions. This study also focuses on synthesizing a novel MOF using the OBA ligand coordination to the aluminium metal center to form stable 3-D framework systems to catalyze the major organic reactions. Understanding structure–activity correlations, metal–ligand collaboration, and the function of framework porosity in promoting reactant diffusion and product formation are all given consideration. The findings demonstrate the efficacy of tailored MOF structures as reliable and reusable heterogeneous catalysts for organic transformations that are significant to industry and the environment.

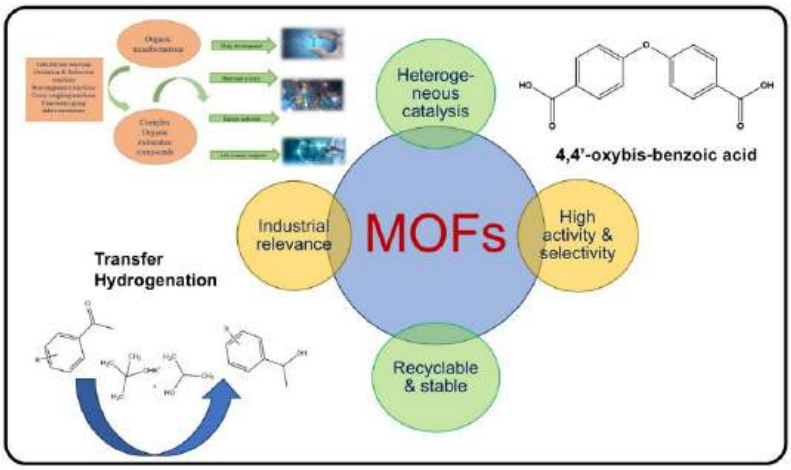

Fig. 1. MOF-based Catalytic systems for industrially important organic reactions

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CCS - D4 - P25
Dehydrogenation of methanol to methyl formate using $CuO/CuAl_2O_4/Al_2O_3$-catalysts

Bastian Schaal[1], Doreen Kaiser[1], Martin Bertau[1]
[1]TU Bergakademie Freiberg, Germany

The dehydrogenation of methanol to methyl formate is a promising alternative to the carbonylation of methanol with carbon monoxide. Mostly Cu-bearing catalysts are used for the dehydrogenation of methanol, yielding 22 – 36 % of methyl formate in a temperature range of 200 – 310 °C.[1] We investigated 3 different catalyst compositions (40, 50 and 60 mol% CuO with 60, 50 and 40 mol% Al_2O_3 respectively) at three different calcination temperatures (800, 950 and 1100°C), which led to nine different catalysts comprised of CuO, $CuAl_2O_4$, $CuAlO_2$ and Al_2O_3. The catalysts were prepared by coprecipitation of copper and aluminium citrate. The $CuO/CuAl_2O_4/Al_2O_3$-catalysts were tested for the methanol dehydrogenation at 210, 240 and 270 °C without prior reduction. CuO undergoes rapid reduction to Cu^0 under the reaction conditions while $CuAl_2O_4$ slowly releases Cu^0 and Al_2O_3. The highest methyl formate yield of 30 % is achieved at 270 °C with a catalyst composition of 60 mol% CuO and 40 mol% Al_2O_3 and a calcination temperature of 800 °C. If the calcination temperature increases to 950 °C, the yield decreases to 25 % but the methyl formate selectivity rises from 51 to 89 %. The methyl formate yield increases to 35 - 40 % after 15 h of reaction time because the conversion increases due to the slow reduction of $CuAl_2O_4$. After 24 h the yield decreases to 30 % due to selectivity increases for dimethyl ether and carbon monoxide. This equals 83 % of the equilibrium methyl formate yield of 36 % at 240 °C reaction temperature.

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The 10th EuChemS Chemistry Congress

12 - 16 July 2026

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Posters

Energy, Environment & Sustainability (EES)

EES - D1 - P01
Mechanistic insights into charge and energy transfer from first-principles calculations

Anna Leo[1], Andrea Peluso[1]
[1]Dpto di Chimica e Biologia "Adolfo Zambelli", Università di Salerno, Italy

Photovoltaic technologies provide a scalable route for direct solar-to-electric energy conversion, with organic solar cells (OSCs) offering chemically tunable electronic properties, low-cost fabrication, and mechanical flexibility compared to inorganic devices.[1,2] Despite recent advances pushing bulk heterojunction (BHJ) OSC power conversion efficiencies to ~19.5%, [3,4] commercialization is hindered by low open-circuit voltages. Given the wide optical bandgap of OSCs, this voltage losses reflect the presence of efficient non-radiative decay pathways, whose suppression is critical for achieving competitive performance.
Device efficiency is determined by the interplay of elementary processes at the donor–acceptor interface, including photoinduced charge transfer, energy transfer, and recombination. Accurate, predictive evaluation of the rates of these processes is essential for rational materials design.
Herein, we introduce a fully quantum mechanical, first-principles framework capable of reliably predicting radiative and non-radiative transition rates at affordable computational cost.[5] The approach combines Fermi's Golden Rule with nuclear coordinates and vibrational properties derived from density functional theory (DFT) calculations, enabling direct evaluation of transition rates without empirical fitting.[6]
Application to small molecules and large molecular systems, demonstrates excellent agreement with experimental data[7] and provides mechanistic insight into the microscopic origin of non-radiative decay offering a predictive strategy for designing next-generation organic semiconductors with intrinsically suppressed energy losses.

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EES - D1 - P02
Ultrafast laser-driven fabrication of NiCoFe carbides for exceptional oxygen evolution reaction

Muhammad Aurang Zeb Gul Sial[1], Mohammad Qamar*[1,2]
[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Materials Science and Engineering Dept., King Fahd University of Petroleum and Minerals, Saudi Arabia

Developing cost-effective, highly efficient, and durable electrodes is pivotal for advancing electrochemical water splitting, particularly the oxygen evolution reaction (OER). Herein, a nickel cobalt iron (NiCoFe) carbide supported on nickel foam is synthesized by using direct laser writing. The laser-induced NiCoFe carbides feature distorted crystal lattices with disrupted atomic arrangements, setting them apart from conventional structures. These carbides demonstrate exceptional OER activity, achieving a lower overpotential than commercial IrO_2 to reach 10 mA cm^{-2} in alkaline solutions. The defective surface significantly enhances the adsorption of critical intermediates, namely, OH*, O*, and OOH*, during the OER processes. Density functional theory calculations reveal that these surface defects accelerate electron transfer, inducing charge redistribution at the interface and reducing the energy barrier of the rate-determining step to 0.97 eV. This study underscored the transformative role of surface defects at the electrocatalyst interface, offering valuable insights into designing electrode materials for an efficient electrochemical reaction.

Acknowledgments: The authors express their gratitude for the financial support received from the Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRCHTCM) at King Fahd University of Petroleum and Minerals (KFUPM), specifically under project # INHT2414.

EES - D1 - P03
Fluorescent nanolignin for coupled sensing-reduction of hexavalent chromium in aqueous matrices

Vinicius Sarracini Santos[1], Gustavo Metzker[1], Isabela Carreira Constantino[1], Antonio Carlos Roveda Júnior[2], Valmor Roberto Mastelaro[2], Márcia Cristina Bisinoti[1], Altair Benedito Moreira[1]
[1]São Paulo State University, Brazil; [2]University of São Paulo, Brazil

The high generation of agro-industrial by-products has attracted attention in studies focused on the valorization and application of these residues. In this context, nanolignin is highlighted, defined as a lignin-derived nanomaterial has emerged as a promising material due to its diversity of applications. However, its fluorometric properties remain underexplored. [1] Additionally, toxic metallic ions, such as Cr(VI), presents high concern to environmental and human health, requiring constant monitoring in diverse environmental compartments.[2] In this study, fluorescent nanolignin was hydrothermally synthesized using accessible reagents. The resulting nanoparticles sized from 50 to 350 nm with oxygen-containing groups, including characteristic constituents of lignin: guaiacyl, syringyl and *p*-hydroxyphenyl as confirmed by FTIR analysis. The nanolignin presented high intensity and sharp and well-defined fluorescence with $\lambda_{excitation}$ = 230 nm. Studies involving 12 interferents showed that nanolignin had high selectivity for Cr(VI) fluorometric detection, with $\lambda_{excitation}$ = 340 nm being the most selective wavelength for this ion. The method validation showed linear correlation (R^2=0.98), with limits of detection and quantification of 0.38 and 1.18 µmol L^{-1}, respectively. No matrix effects were observed in ultrapure water, tap water, groundwater and bottled water. These results are comparable to standard colorimetric method. The sensing mechanism was investigated using GC-MS and XPS, revealing the reaction of Cr(VI) with aromatic compounds present in nanolignin. This interaction decreases the conjugation of aromatics, explaining the observed fluorescence quenching. In this reaction, Cr(VI) is reduced to Cr(III), a 300-fold less toxic specie, presenting combined environmental sensing and remediation applications.

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EES - D1 - P04
Dimethyl Ether (DME): From sustainable production to green applications in the low-carbon economy

Dong Jin Suh[1], Won-jun Cho[2]
[1]Wooi Plant Co., Ltd., Republic of Korea; [2]Bio Friends Inc., Republic of Korea

Dimethyl Ether (DME, CH_3OCH_3) is rapidly emerging as a multi-functional low-carbon platform molecule and energy carrier essential for achieving global decarbonization goals. Beyond its role as a clean-burning alternative fuel, DME offers exceptional versatility as a hydrogen carrier, green chemical intermediate, and environmentally benign extraction solvent and propellant.
This study highlights DME's comprehensive contribution to the transition toward a circular, low-carbon economy, emphasizing two main pillars. (1) Sustainable production pathways: DME can be synthesized from diverse and renewable feedstocks, including biomass-derived syngas (BioDME) and captured CO_2 with renewable H_2 via Power-to-X technologies. These routes enable feedstock-flexible, carbon-neutral production of a clean liquid fuel and chemical intermediate. (2) Versatile decarbonization applications: As an ultra-clean fuel, DME possesses a high cetane number (55–60) and combusts with near-zero particulate and SO_x emissions. It also functions as a hydrogen-storage medium and precursor for value-added chemicals such as acetic acid and olefins, while serving as a safe and eco-friendly solvent and aerosol propellant in industrial applications.
In this presentation, recent R&D and pilot-scale demonstrations conducted in the Republic of Korea are briefly introduced, focusing on sustainable DME synthesis technologies and novel extraction systems utilizing DME for high-moisture biomass residues. These systems enable direct recovery of valuable compounds without energy-intensive drying, offering new routes to produce bio-based fine-chemical products under mild and environmentally safe conditions.
By integrating renewable carbon sources with such advanced utilization technologies, DME acts as a crucial bridge linking sustainable production to multi-sectoral decarbonization, reinforcing its pivotal role in building a resilient and carbon-neutral energy future.

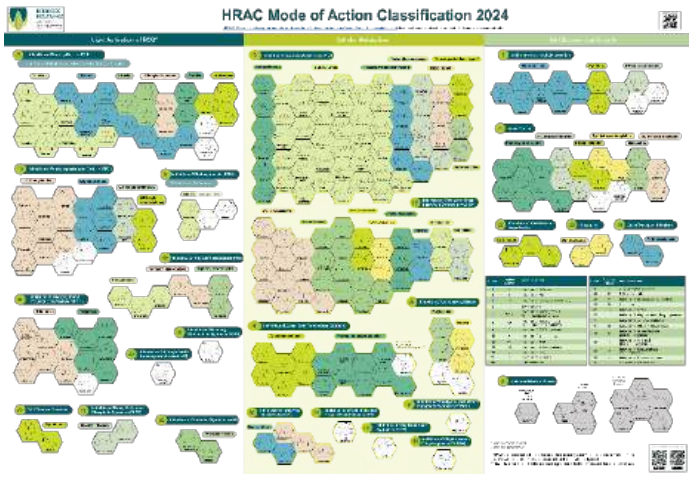
Acknowledgements: This research was supported by the Energy Efficiency & Resources Core Technology Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP), funded by the Ministry of Trade, Industry and Energy (MOTIE) of Korean government under grant No. 20224000000440.

EES - D1 - P05

The new HRAC herbicide mode of action classification 2026 - An essential contribution to sustainable agrochemistry

Jens Frackenpohl[1], Jonathan F. Schmelzer[2]
[1]Bayer AG, CropScience Division, Profile Driven Chemistry, Germany; [2]Goethe Universität Frankfurt, Fachbereich Geographie, Germany

Herbicides are a key tool for sustainable and efficient agriculture with strong positive impact on soil conservation as well as quality and quantity of harvested crops. Although herbicides remain the most effective solution for weed control, they face multiple challenges, such as the emergence and growth of resistant weed populations. Thus, it is essential that crop protection research acts rapidly to provide farmers with new solutions that enable them to fight back against resistant weed species and to secure global food production.
HRAC Global strives to promote Integrated Weed Management encompassing chemical, cultural, biological and mechanical measures to avoid herbicide resistance. Using different mode of action (MoA) chemistries is an important measure to circumvent weed resistance development as much as possible. The new HRAC Herbicide MoA Classification poster provides an updated overview on the available herbicide chemistries. The HRAC Global Herbicide MoA Working Group reviewed literature information, sales data, biological results and their relevance for resistance management for the latest edition of the presented poster. It serves as a valuable tool for scientific exchange and for guidance with respect to resistance management.



Examples:

1. In contrast to other modes of action emerging resistance against inhibitors of acyl-acyl carrier protein thioesterase (FAT) has not been discussed broadly making it an attractive target for identifying new herbicides.[1,2] Recently, it has been shown that several herbicides, so far with unknown mode of action, control weeds due to inhibition of FAT.[3-7] Thus, commercially available FAT-inhibitors have been added as the new class 30 to the HRAC poster which will be discussed in detail.
2. Based on new research results MoA classifications are reviewed and adapted on a regular basis. Likewise, members of HRAC groups 3 (Inhibition of tubulin assembly) and 23 (Inhibition of microtubule organization) have been re-allocated and new members[8] have been taken up.

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EES - D1 - P06

Hydrophilic bipyridine–sulfonate polymeric colloids as stable redox electrolytes for aqueous organic flow batteries

Muhammad Zeeshan[1], Shakira Allah Baksh[1], Shahid Ali[2], Safyan Akram Khan[2], Ata-ur-Rehman[2], Muhammad Nawaz Tahir[1,2], Muhammad Mansha[2]*, Majad Khan[1,2]*

[1]Dept. of Chemistry, College of Chemical Sciences, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals, Saudi Arabia

** Email: manshachohan@kfupm.edu.sa (Muhammad Mansha) majad.khan@kfupm.edu.sa (Majad Khan)*

Aqueous organic redox flow batteries (AORFBs) require stable and high-capacity redox-active materials to advance sustainable energy storage technologies. In this work, we present hydrophilic polymeric colloids, Poly(bis(4-vinylphenyl)-[2,2′-bipyridine]-4,4′-dicarboxamide)-co-(sodium 4-vinylbenzenesulfonate) (P1 and P2), incorporating bipyridine redox centers and sulfonated aromatic groups. These copolymers were synthesized via controlled precipitation and dispersion polymerization, forming crosslinked colloidal networks that self-assemble into water-dispersible particles (~500 nm). Structural and compositional analyses (FTIR, $^{1}H/^{13}C$ NMR, and elemental analysis) confirmed successful copolymer formation, while FESEM and DLS revealed uniform, stable colloidal morphologies. Electrochemical characterization demonstrated fully reversible redox behavior of the bipyridine moieties in 1 M KOH, with well-defined redox couples and excellent cycling retention. When integrated as anolytes in laboratory-scale flow cells (with ferri/ferrocyanide catholyte and Nafion N424 separator), P1 and P2 achieved discharge capacities of 89 mAh L^{-1} and 142 mAh L^{-1}, respectively, sustaining > 75 and > 200 cycles with minimal capacity fade. The colloidal architecture effectively suppresses active-species crossover, enabling use of low-cost porous membranes. This study demonstrates a robust, scalable, and metal-free platform for high-voltage AORFBs, linking molecular redox design to durable colloidal electrolyte performance for next-generation electrochemical energy storage.

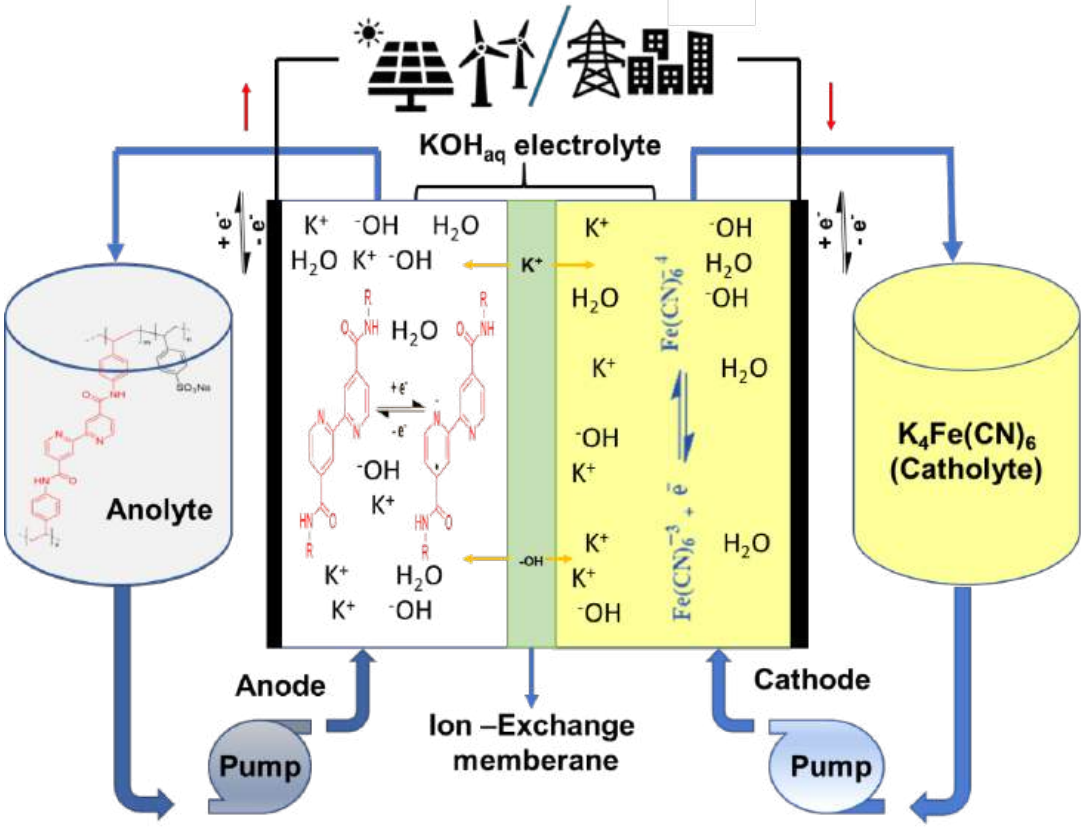

Fig. 1. Graphical Abstract

Acknowledgement: The Authors would like to acknowledge the support and facilities provided by IRC-HTCM, KFUPM.

EES - D1 - P07
Overcoming trade-offs in thick sulfur cathodes for lean Li–S batteries

Sun-Sik Kim[1], Hee-Jun Kim[1], Hun-Seong Kim[1], Jaewon Lee[1], Hyun Young Jung[1,2]
[1]Dept. of Energy System Engineering, Gyeongsang National University, Republic of Korea; [2]Dept. of Energy Engineering, Gyeongsang National University, Republic of Korea

Lithium-sulfur (Li-S) batteries, with a theoretical energy density of 2567 Wh kg^{-1}, have drawn significant interest for use in fields such as aviation and portable electronics. Yet, their real-world applicability hinges on achieving extensive sulfur conversion and reconversion when operating with high sulfur areal loadings (S_{load} > 3 mg cm^{-2}) and restricted electrolyte amounts (E/S < 8 µL mg^{-1})[1]. Using a low volume of electrolyte enhances energy density but also significantly restricts ion access to deeply embedded sulfur, leading to sluggish ion transport, increased polarization, and severe interfacial ion imbalances in thick sulfur cathodes[2]. These challenges critically hinder sulfur electrokinetics under lean electrolyte conditions[3]. In this study, we introduce an ion trade-off strategy that mitigates interfacial ion imbalance by incorporating a cation-conductive active binder. This binder enables continuous lithium-ion exchange near regions with limited electrolyte infiltration, thereby forming an ion-rich sulfur-binder-electrolyte interface[1]. The dynamically formed ionic interface reactivates previously inaccessible sulfur, contributing to additional capacity while reducing both ion transport and charge transfer resistance. Utilizing this approach, sulfur cathodes with a high areal loading of 8.1 mg cm^{-2} and an electrolyte-to-sulfur (E/S) ratio of 6 µL mg^{-1} achieved 60.89% sulfur utilization, delivering a capacity of 1020 mAh g^{-1}. Furthermore, a lean-electrolyte Li-S pouch cell assembled with this strategy achieved a high energy density of 324 Wh kg^{-1}, validating the effectiveness of interfacial ion trade-off in overcoming transport limitations. This work presents a promising direction for designing thick electrodes in next-generation high energy density battery systems.

Acknowledgements: This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2024-00352398).

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EES - D1 - P08
Boosting electrochemical performance of $LiFePO_4$ through carbon layer control

Yong Joon Park[1]*, Da Eun Kim[1]
[1]Dept. of Advanced Materials Engineering, Graduate School Kyonggi University, Republic of Korea

Lithium iron phosphate ($LiFePO_4$, LFP) is widely utilized in electric vehicles and energy-storage applications due to its excellent safety and structural stability. Nevertheless, its inherently low electronic conductivity and limited lithium-ion mobility continue to restrict its rate performance. To address these challenges, carbon coating has been extensively adopted, yet the quality and functional properties of the coating layer remain strongly dependent on the choice of carbon sources and the structural characteristics of the resulting carbon. The primary objective of this study was to establish an optimized carbon-coating strategy that simultaneously increases the carbon yield and enhances the structural quality of the coating layer. To achieve this, we explored a mixed carbon-source system based on glucose and polystyrene, aiming to leverage their complementary characteristics—namely, the uniform coating behavior of glucose and the high carbon content of polystyrene. Additionally, ferrocene was introduced as a catalytic additive to promote graphitization during thermal treatment, enabling refinement of the coating structure without relying on high-temperature processes. The experimental approach involved synthesizing LFP/carbon composites through a solid-state reaction route, followed by systematic variation of glucose-to-polystyrene ratios and controlled addition of ferrocene. Structural and morphological characteristics of the carbon coatings were examined using transmission electron microscopy, Raman spectroscopy, and carbon–sulfur analysis. Electrochemical characterization was conducted using galvanostatic cycling, impedance spectroscopy, and GITT to evaluate how the engineered carbon layers influence charge-transfer behavior and ion-transport pathways. Overall, this work provides a comprehensive framework for designing carbon coatings with improved structural quality and efficient precursor utilization, offering a scalable route for enhancing the electrochemical functionality of LFP cathodes.

Acknowledgements: This study was supported by the Materials and Components Technology Development Program (grant No.20024249) and Technology Innovation Program (grant No. RS-2024-00427225) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea).

EES - D1 - P09
Upcycling industrial solid waste into a high-efficiency adsorbent for sustainable water treatment

Oumaima Aqil[1], Mohammed Chafi[2], Saloua Jemjami[1]
[1]Faculty of Sciences and Techniques of Settat, Hassan I University, Morocco; [2]Higher School of Technology of Casablanca, Morocco

The growing demand for efficient and sustainable water treatment technologies has intensified interest in converting industrial solid waste into value-added functional materials[1]. In this work, an industrial by-product was upcycled into a high-efficiency adsorbent through a chemical activation route, aiming to enhance surface functionality and adsorption performance. The physicochemical properties of the treated material were characterized using XRD, FTIR, SEM and XRF analyses, confirming the development of a more porous structure and the introduction of active surface sites favorable for pollutant capture[2].
Adsorption experiments were carried out using representative organic pollutants commonly found in contaminated effluents[2]. The treated material exhibited significantly improved adsorption capacities compared to the raw precursor, with rapid uptake kinetics and strong affinity toward persistent contaminants. The effects of pH, contact time, initial concentration, and temperature were also investigated to elucidate the adsorption mechanisms involved[2].
The results demonstrate that converting industrial waste into functionalized adsorbents offers a promising, low-cost and environmentally responsible alternative for sustainable water treatment[3]. This research highlights the potential of waste-derived materials to contribute to circular economy strategies while providing efficient solutions for pollutant removal.

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EES - D1 - P10

CO_2 hydrogenation to ethanol over alkali-promoted trimetallic catalysts in a packed-bed reactor

Andrii Kostyniuk[1]*, Blaž Likozar[1]
[1]National Institute of Chemistry, Dept. of Catalysis and Chemical Reaction Engineering, Slovenia
**andrii.kostyniuk@ki.si*

The efficient valorisation of CO_2 into higher value products is a key strategy for mitigating greenhouse gas emissions and enabling sustainable chemical production. Direct CO_2 hydrogenation to ethanol is particularly attractive, yet it remains challenging due to limited selectivity and productivity of most catalytic systems[1]. Here, we demonstrate a highly active and stable series of alkali-promoted trimetallic catalysts for gas-phase CO_2 hydrogenation to ethanol in a continuous packed-bed reactor (Fig. 1). Catalysts with varying Cs loadings (xCs/CuZnFe) were synthesised and systematically evaluated. The optimal formulation, 4%Cs/25%Cu–25%Zn–50%Fe, achieved 5.0 mmol·gcat^{-1}·h^{-1} ethanol STY at 300 °C and 20 bar, with H_2/CO_2 = 3 and GHSV = 9917 h^{-1}, representing one of the highest reported space-time yields among non-noble metal catalysts[2]. The corresponding CO_2 conversion reached 17%, while C_2^+ alcohol selectivity was 78.8 mol%, surpassing most literature benchmarks. These performance enhancements were attributed to synergistic interactions between Cs, Cu, Zn, and Fe, producing high oxygen vacancy density, optimal basicity, and enlarged pore diameters which collectively facilitated CO_2 activation and C–C coupling. Catalyst structure and surface chemistry were analysed using XRD, BET, SEM/STEM-EDX, XPS, CO_2-TPD, ICP-OES, and in situ DRIFTS, revealing that 4 wt% Cs loading prevents Cu loss, enhances crystallinity, and stabilises active sites. The mechanistic investigation showed a tandem pathway involving both CO insertion and formate routes, with the formate pathway dominating. Notably, an excess of Cs (8 wt%) increased basicity and CO_2 adsorption, but hindered ethanol selectivity due to stronger binding and side reactions. This study demonstrates that precise alkali promotion of trimetallic catalysts enables efficient CO_2-to-ethanol conversion, providing new insight into catalyst design for scalable, sustainable fuel and chemical synthesis.

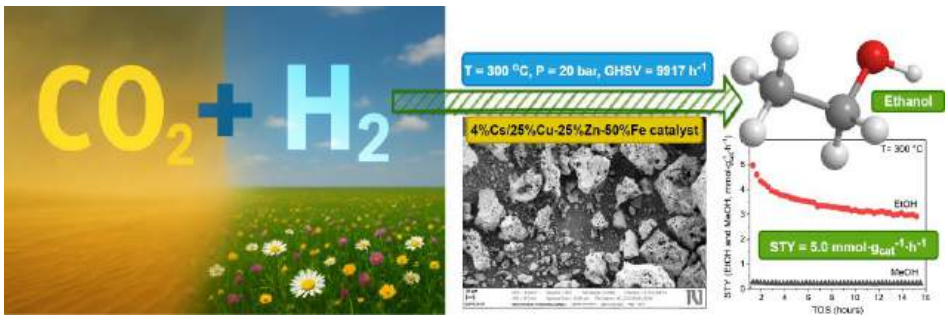

Fig.1. Schematic representation of CO_2 hydrogenation to ethanol over a high-performance catalyst.

Acknowledgements: This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreements No. 101221903, 101214604, and 101086411. The views and opinions expressed are those of the author(s) only and do not necessarily reflect those of the European Union or the European Innovation Council and SMEs Executive Agency (EISMEA). Neither the European Union nor the granting authority can be held responsible for any use that may be made of the information contained herein. The authors also gratefully acknowledge the financial support of the Slovenian Research Agency (ARIS) through the research grant J7-4638 (Unlocking the selective catalytic conversion processes of CO_2 to ethanol – UliSess).

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EES - D1 - P11

Development of plant growth-promoting bacteria with artificial humic acids capsules for enhanced agricultural sustainability

Robert Guiu-Sans[1,2], Bartosz Tylkowski[1], Magdalena Jopek[3], Paweł Trzciński[4], Svitlana Filonenko[5], Nataliia Doskaliuk[5], Ricard Garcia-Valls[2], Joseph J. Richardson[6], Magdalena Olkiewicz[1]

[1]Eurecat, Centre Tecnològic de Catalunya, Chemical Technologies Unit, Spain; [2]Dept. of Chemical Engineering, Universitat Rovira i Virgili, Spain; [3]Intermag sp. z o.o., Poland; [4]Instytut Ogrodnictwa - Państwowy Instytut Badawczy, Zakład Mikrobiologii i Ryzosfery, Poland; [5]Humify GmbH, Germany; [6]Dept. of Chemical and Environmental Engineering, School of Engineering, RMIT University, Australia

Massive agricultural production is required to feed the increasing global population. However, the current extensive use of agrochemicals pollutes the environment.[1] Therefore, new crop performance enhancers need to be developed. In their design, plant biostimulants become essential.

Plant biostimulants are substances or microorganisms applied to plants to enhance their growth, regardless of their nutrient content.[2] A promising subset is humic substances, which are constituent fractions of soil organic matter and are biologically active.[3] Another strong candidate is plant growth-promoting bacteria (PGPB), an important biological alternative with the capacity to increase crop yield.[3]

Encapsulation of the biostimulants aims to protect and deliver them efficiently, minimising environmental disruption and loss of costs, while displaying synergistic effects. Nevertheless, current encapsulation techniques in agriculture often involve the use of non-biodegradable materials,[4] and costly processes.[5]

In this study, sustainable biostimulant capsules, based on biodegradable polymer (alginate), loaded with artificial humic acids (AHAs) and different species of PGPB, are prepared by ionic gelation. Once obtained, the formulations will be tested in field trials to evaluate their efficacy.

Robert Guiu Sans is a fellow of Eurecat's "Vicente López" PhD grant program.

The authors acknowledge financial support from the European Union's Horizon Europe research and innovation programme under grant agreement 101157265.

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EES - D1 - P12
Engineering nitrogen-enriched covalent organic framework for carbon capture

Aasif Khan[1*], Aasif Helal[1]
[1]King Fahd University of Petroleum and Minerals, Saudi Arabia

The continuous rise in atmospheric carbon dioxide (CO_2) concentrations has become a critical driver of global environmental challenges, including climate change and global warming. Developing efficient and sustainable carbon capture technologies is therefore imperative. Carbon capture and utilization (CCU) offer a promising route, enabling the transformation of captured CO_2 into valuable chemical products. Covalent organic frameworks (COFs) have emerged as a versatile class of porous crystalline materials, characterized by tunable porosity, high surface area, structural diversity, and exceptional thermal and chemical stability. These properties make COFs attractive candidates for carbon management applications. Their chemical flexibility further allows the incorporation of functional groups-such as amines, heteroatoms, or polar moieties that selectively interact with CO_2 molecules through acid-base interactions or hydrogen bonding.
In this work, we focus on the rational design and synthesis of nitrogen-enriched COF materials to enhance CO_2 capture and utilization efficiency. Nitrogen incorporation within the COF framework significantly improves selective adsorption performance. The synthesized materials were comprehensively characterized using advanced spectroscopic techniques to confirm their structural integrity and functional properties. Realizing the full potential of COFs in practical carbon management will require synergistic efforts across materials chemistry, process engineering, and computational modeling. Such interdisciplinary collaboration is essential to advance COFs from laboratory innovation to scalable solutions for sustainable carbon capture and utilization.

EES - D1 - P13

Synthesis of nickel-based catalysts for the (photo)thermocatalytic production of γ-valerolactone

Jordi Rigual-Miret[1,2], Arnau Fons[3,4], Josep Nogués[3,5], Elvira Gómez[1,2], Borja Sepúlveda[4], Albert Serrà[1,2]
[1]Grup d'Electrodeposició de Capes Primes i Nanoestructures (Ge-CPN) – Universitat de Barcelona, Spain; [2]Institute of Nanoscience and Nanotechnology (IN²UB) - Universitat de Barcelona, Spain; [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Spain; [4]Institut de Microelectrònica de Barcelona (IMB-CNM, CSIC), Campus UAB, Spain; [5] ICREA, Spain

Biomass is the most abundant renewable energy source on the planet and represents an emerging alternative to fossil fuels, supporting the global transition toward sustainable energy systems capable of mitigating climate change. Among the wide variety of products obtainable from biomass, some compounds are of particular interest for their industrial applications as biofuels or green solvents, including γ-valerolactone (GVL). GVL is a versatile, biodegradable, and non-toxic platform molecule with applications in energy storage, fuel additives, polymer synthesis, and fine chemical production, making its sustainable large-scale production a strategic objective for the bioeconomy. However, its synthesis is still limited by the high energetic and economic costs associated with current catalytic systems.

This study investigates the preparation of nickel-based catalysts via electroless deposition -an industrially scalable technique- and the use of 2-propanol (IPA) as an in-situ hydrogen donor for the hydrogenation of levulinic acid (LA) to GVL. The synthesized materials were evaluated under thermal, photothermal, and photocatalytic conditions using conventional heating, near-infrared (NIR) irradiation, and concentrated solar illumination both using pure and real biomass hydrolysates.

Light-driven NIR activation consistently outperformed conventional thermal treatments, achieving almost quantitative LA conversion (>99.9%) and GVL selectivity (>99%), with negligible metal leaching (ppb range) after five reaction cycles. Solar-concentrator experiments confirmed that the catalysts operate effectively under real sunlight, maintaining high activity and selectivity. Tests using real biomass hydrolysates further demonstrated the robustness of the Ni-based catalysts in complex reaction matrices.

Overall, these findings show that Ni-based catalysts can rival noble-metal systems while effectively exploiting in-situ hydrogen donors such as IPA. This work positions solar photo-thermocatalysis as a practical and scalable pathway for the sustainable valorization of biomass.

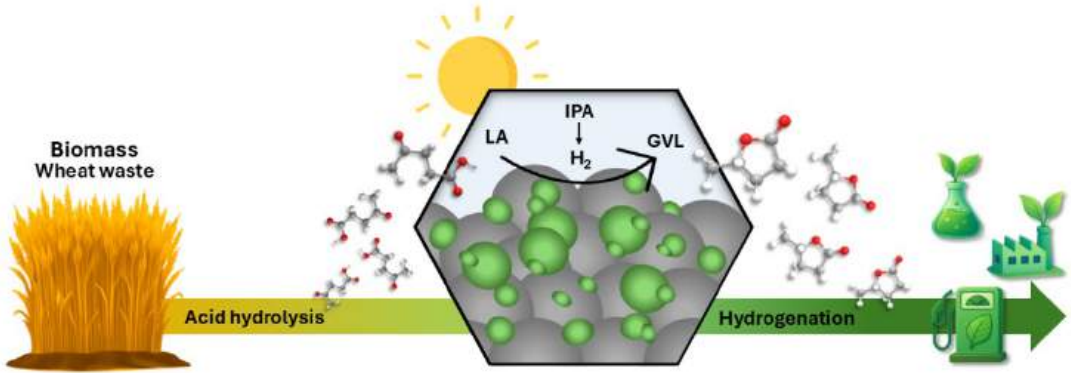


Fig. 1. Schematic representation of the photo-thermocatalytic conversion of levulinic acid to GVL under solar illumination on Ni-based catalysts.

Acknowledgements: The authors would like to express their gratitude to the *Departament de Recerca i Universitats*, particularly the *Departament d'Acció Climàtica, Alimentació i Agenda Rural*, as well as *the Fons Climàtic de la Generalitat de Catalunya* (project 2023 CLIMA 00009 AGAUR).

EES - D1 - P14

Entropy management of PLA: Novel state-based screening method for decision-support from feedstock to end-of-life treatment

Britt Segers[1], Philippe Nimmegeers[2], Cristina Moyaert[1], Pieter Billen[1]
[1]iPRACS, University of Antwerp, Belgium; [2]EnvEcon, University of Antwerp, Belgium

Biomass is widely recognised as an alternative to fossil-based resources, yet its implementation remains challenging. Diverse feedstocks and numerous potential end products, often involving non-commercial conversion processes, limit the applicability of current assessment methods. At low technology readiness levels (TRL), data unavailability makes process based assessment methods such as life cycle assessments (LCA) and techno-economic assessments (TEA) impractical due to the required extensive inventories and predefined conditions.
To address this, we propose an initial screening tool based on state variables, focusing on the beginning and end states of the process. This eliminates the need for detailed process-specific data and supports early decision-making consistent with circularity principles.
Energy is identified as the dominant factor, influencing both TEA costs and global warming potential (GWP) in LCA. Two state variables are identified to capture the energy-related impacts: statistical entropy and carbon oxidation states. Statistical entropy, as defined by Shannon and adapted by Rechberger and Brunner for material flow analysis, is here extended to link entropy with energy requirements. Two entropy types were considered: compositional (differences between feedstocks and end of life (EoL) products) and geospatial (distribution of feedstock). Carbon oxidation states provide a stable indicator of EoL product value, independent of market fluctuations.
This methodology is applied to polylactic acid (PLA), a bio-based, biodegradable polymer with strong potential to replace fossil-based plastics. Key considerations include feedstock sourcing, where location, availability and composition play critical roles, and EoL treatment options. While PLA is compostable, alternatives such as combustion, mechanical recycling, and chemical recycling may offer better outcomes.
This approach enables early-stage decisions in biopolymer development, integrating feedstock sourcing and EoL strategies to support circularity.

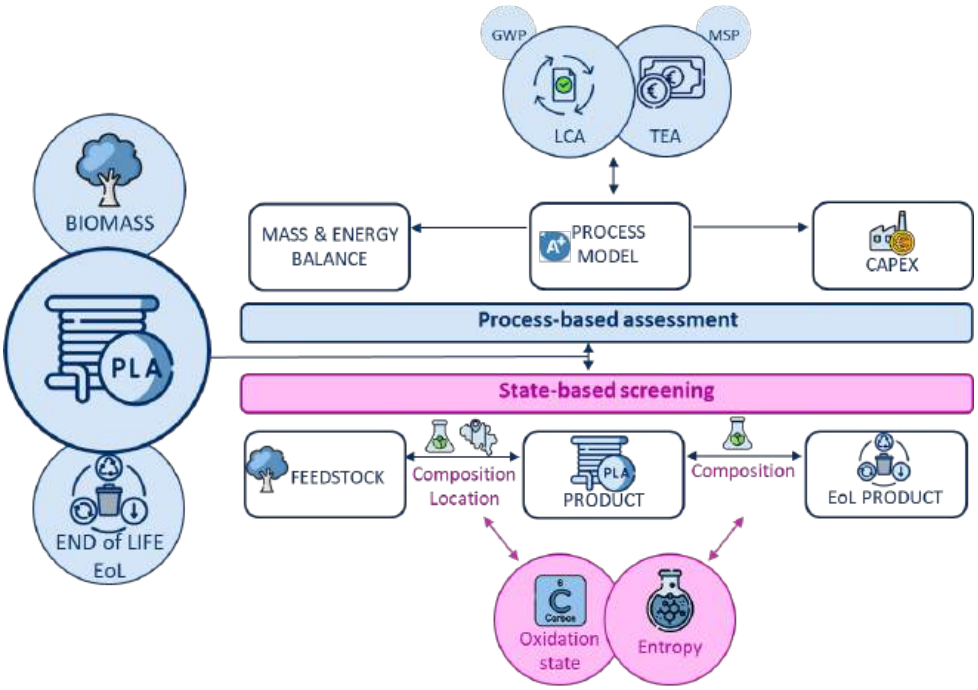


Fig. 2. Introduction of a novel state-based screening method to guide decision-making consistent with process-based assessments applied to the production and end of life of polylactic acid (PLA)

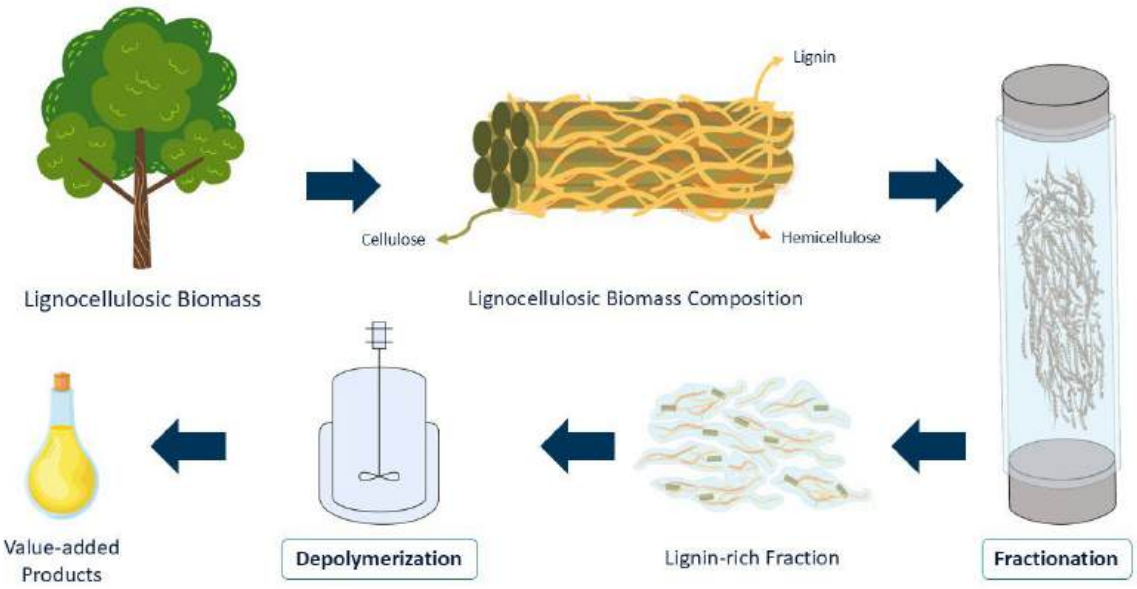
EES - D1 - P15

An integrated biorefinery approach for sustainable fuel production via low-pressure flow-through organosolv fractionation and catalytic lignin upgrading

Imam Hidayat Nurwahid[1,2], Won Yeong Lee[1,3], Sarah Keiza Ismail[1,2], Ye-jin Lee[1,4], Chang Soo Kim[1,2]
[1]Korea Institute of Science and Technology (KIST), Republic of Korea; [2]University of Science and Technology (UST), Republic of Korea; [3]Inha University, Republic of Korea; [4]Korea University, Republic of Korea

Environmental concerns about the depletion of fossil resources have accelerated the transition toward a circular bioeconomy based on lignocellulosic biomass (LCB). Although LCB is a globally abundant carbon source, its comprehensive utilization remains limited due to its structural robustness and the deficiencies of conventional pretreatment strategies.[1] Efficient lignin valorization is critical for the economic feasibility of biorefineries. However, standard methods typically employ harsh conditions that significantly reduce the chemical reactivity of lignin.[2] This study proposes an integrated two-step biorefinery approach to overcome these challenges. First, a low-pressure flow-through organosolv fractionation system was developed to isolate high-purity reactive lignin. Unlike batch systems, the flow-through design minimizes residence time and prevents lignin condensation, thereby preserving β-O-4 linkages, the most abundant and crucial aryl ether bonds in lignin.[3] Second, the fractionated lignin underwent catalytic depolymerization using a Pt/Al_2O_3 catalyst in a biphasic water-tetralin solvent system. The cooperative effect between the platinum active sites and the acidic alumina support facilitated selective C-O bond cleavage.[4] Simultaneously, tetralin served as a hydrogen-donating radical scavenger, thereby inhibiting coke formation and stabilizing reactive intermediates.[5] This integrated system maximizes the production of valuable phenolic compounds and sustainable fuels, representing a significant advancement toward the comprehensive valorization of low-value biomass into high-value aromatic products.

Graphical abstract:



Acknowledgements: KIST Institutional Program (2E33931, 2E33852).

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EES - D1 - P16
Mechanically assisted synthesis and application of catalyst for hydrogen generation

Kent Kütt[1], Indrek Niinemets[1], Martin Jürisoo[1], Kerli Liivand[2], Moonika Ferschel[1], Dmitri Shushtchik[1], Eduard Pihl[1], Olga Pihl[1], Allan Niidu[1]
[1]TalTech Virumaa College, Estonia; [2]NICBP, Estonia

A mechanically assisted synthesis of ZIF-8[1] was developed to produce precatalyst material for hydrogen generation in two-stage thermal treatment unit.[2] Produced ZIF-8 was calcined under Ar atmosphere at 370°C while retaining its structural integrity as shown by PXRD measurements. Thus obtained solid material was mixed with MgO and used as cracking catalyst in the second stage of thermal treatment unit or in the condenser head (see Table 1). Used oil in admixture with RDF was used as feedstock for the current project giving 544-834 m^3 H_2/t feed while the inclusion of catalyst in the cracking column lead to the highest yield for H_2.

	Used 5W40 oil + RDF 0,3:0,7	**Used 5W40 oil + RDF 0,3:0,7**	**Used 5W40 oil + RDF 0,3:0,7**	**Used 5W40 oil + RDF 0,3:0,7**
T, °C	550	550	550	550
Cracking reactor	-	-	-	ZIF8-MgO fr.1
Condenser	-	ZIF8-MgO fr.1	ZIF8-MgO fr.2	-
T, °C	1000	1000	1000	1000
H_2, vol%	64.6	70.77	67.08	71.85
H_2S, vol%	0.59	0.09	0	0
CO_2, vol%	1.6	0.15	0.23	0.23
CO, vol%	13.38	19.36	20.68	19.16
CH_4, vol%	16.84	9.25	11.11	8.46
$C_{xn}H_{yn}$, vol%	2.99	0.38	0.91	0.3
m^3 H_2 / t feed	543.73	732.2	599.7	834.1
m^3 CO / t feed	112.62	200.3	184.9	222.4
H_2 : CO	4.83	3.66	3.24	3.75

Table 1. Gas mixtures produced by two-stage thermal treatment unit.

Acknowledgements: This work was supported through grants ÕÜF16 and ÕÜF18 provided by Estonian Youth and Education Board.

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EES - D1 - P17

Toward selective detection of polycyclic aromatic hydrocarbons using microfluidics paper analytical devices

Mohd Shafiq Nasir[1], Akimitsu Kugimiya[1]
[1]Hiroshima City University, Japan

Polycyclic aromatic hydrocarbons (PAHs) are environmentally persistent pollutants whose field detection is hindered by low concentrations, strong hydrophobicity, and pronounced matrix interferences [1,2]. Microfluidic paper-based analytical devices (μPADs) offer significant potential as promising analytical tools by combining low-cost fabrication, capillary-driven transport, and enzyme-based detection for on-site chemical analysis [3,4]. This work presents a microfluidic paper-based analytical device (μPAD) that integrates supramolecular capture, optimized channel geometry, and enzyme-mediated signal amplification for selective PAH detection. Naphthalene, pyrene, and benz[α]anthracene were selected as model PAHs representing increasing molecular size. Selective capture and separation were achieved using size-matched α-, β-, and γ-cyclodextrins immobilized within microfluidic channels. Host-guest complex formation was confirmed by characteristic peak shifts and intensity changes in UV-Vis absorbance and fluorescence spectra, indicating changes in the electronic environment upon encapsulation. Encapsulation efficiencies were achieved for pyrene, demonstrating strong supramolecular affinity. Systematic geometric studies were conducted to control capillary-driven flow, residence time, and analyte-reagent interactions within multi-channel architectures. Computational fluid dynamics (CFD) simulations were employed to model velocity fields, flow uniformity, and mass-transport behaviour across different designs. The optimized geometry ensured balanced flow distribution and minimized back-flow, and enabled reliable spatial separation of target PAHs. Simulation results showed good agreement with experimental and sensing observations. Signal transduction was achieved using a horseradish peroxidase (HRP)-hydrogen peroxide-tetramethylbenzidine (TMB) system. Practical applicability was demonstrated through spiked recovery experiments using soil samples. Matrix effects were evaluated in the presence of ascorbic acid, toluene, and $CaCl_2$, confirming effective suppression of redox-active, organic, and ionic interferences. Overall, this study demonstrates a sustainable, low-cost, and field-deployable platform for environmental PAH monitoring.

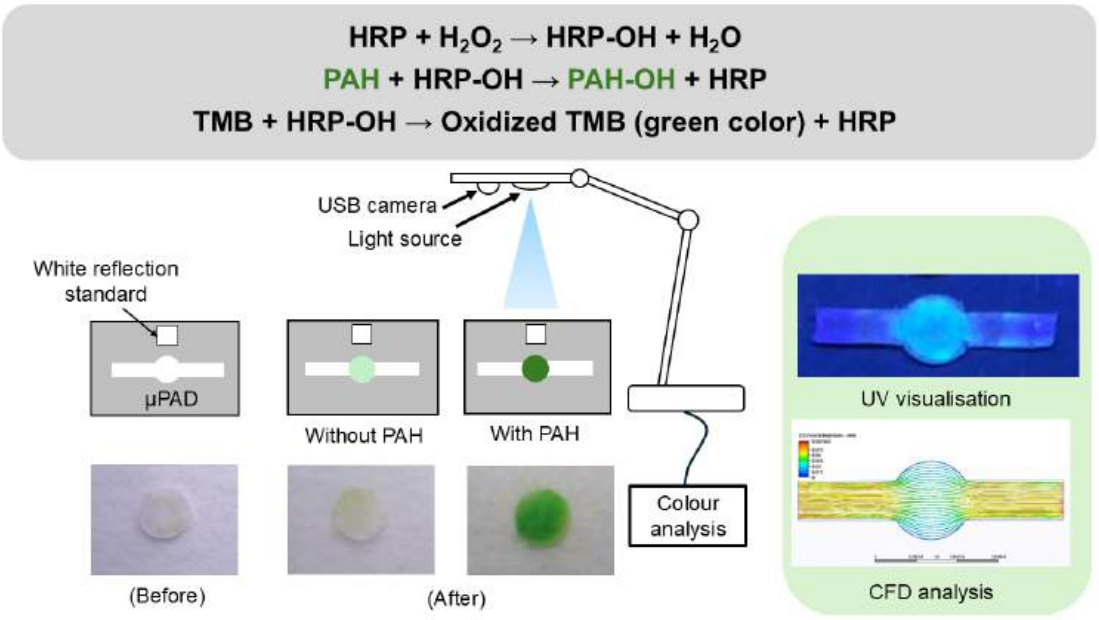

Fig. 1. Experimental set up

This work was partly supported by the Foundation of Chugoku Regional Innovation Research Center, the Japan Research Institute of Industrial Science (Fukuyama), and JSPS KAKENHI Grant Number 25K08827.

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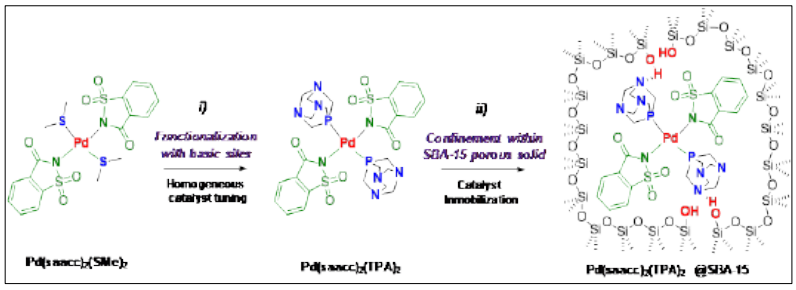
EES - D1 - P18

Pd-Imidate@SBA-15: A multifunctional heterogeneous catalyst for the aqueous room temperature hydrogenation of CO_2 to formic acid

N. Martín[1*], R. Porcar[2], J.L. Serrano[3], J. Pérez[3], P. Lozano[4], F.G. Cirujano[1*], E. García-Verdugo[1*]
[1]Universitat Jaume I, Spain; [2]Universidad Nacional de Educación a Distancia. UNED, Spain; [3]Universidad Politécnica de Cartagena, Spain; [4]Universidad de Murcia, Murcia, Spain
**Corresponding authors: numartin@uji.es; cirujano@uji.es; cepeda@uji.es*

To reduce CO_2 emissions, thermo-catalytic methods should complement electro- and photocatalytic approaches, which face efficiency and scalability issues. Hydrogenation of CO_2 to formic acid, especially using sustainable hydrogen sources, offers a promising solution.[1] Pd-based catalysts, more cost-effective than precious metals, can enhance efficiency if stabilized with water-soluble ligands like PTA. Incorporating Pd into mesoporous silica (SBA-15) improves stability, prevents aggregation, and concentrates reagents near active sites, offering a scalable, efficient system for CO_2 hydrogenation (see Scheme 1).[2]
This work uses cage-like phosphane N-donor ligands (e.g., PTA) to create stable, water-soluble palladium(II) complexes (trans-[Pd(sacc)$_2$(PTA)$_2$]) as single-site catalysts, both homogeneous and within SBA-15 pores. XRD, TGA, UV-Vis, FTIR, N2-physisorption and TEM confirmed the complex confinement within the mesoporous silica. The PTA ligand enhances CO_2 hydrogenation to formic acid/formate by forming HCO_3^- and CO_3^{2-} species, while the Pd-PTA bond prevents Pd aggregation, and the SBA-15 support improves diffusion, as confirmed by ^{1}H-NMR and ^{13}C-NMR.
The incorporation of hydrophilic and basic sites from phosphotriazaadamantane and saccharine in a water-soluble Pd complex and the subsequent confinement into mesoporous silica support increases the activity and stability of the palladium catalytic species for the room-temperature aqueous hydrogenation of either bicarbonate or CO_2 into formic acid. The use of low Pd loadings (0.1%mol) of the well-dispersed complex on SBA-15 mesoporous silica allows performing the reaction under room temperature, and aqueous conditions, exhibiting TON of ca. 50-100, for the CO_2 or bicarbonate hydrogenation, respectively, which is one order of magnitude higher than the homogeneous case, allowing the easy isolation of the solid catalyst, its recycling and the simple purification of the products by centrifugation.



Scheme 1. Design of Pd@Silica as catalysts for CO_2 valorization.

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EES - D1 - P19
Post-combustion CO_2 capture using washcoated structured sorbents

Marleen Rombouts[1], Luca Mastroianni[1], Yoran De Vos[1]
[1]VITO, Coating and Shaping Technologies, Belgium

The European Green Deal sets ambitious targets for greenhouse gas (GHG) emission reduction. Residual, hard-to-abate CO_2 emissions from industrial processes, such as steel production, will need to be captured and, wherever possible, converted into new products. Conventional liquid absorption technologies face major challenges related to high energy demand, environmental impact, and corrosion associated with amine-based solvents. In this context, solid sorbents for CO_2 capture from flue-gas streams holds significant potential to overcome these limitations.
Within the framework of the HE-Carbon4Minerals project, VITO is developing a state-of-the-art mobile CO_2 capture pilot plant for post-combustion capture from diluted industrial flue gases, targeting a capacity of 1 kg CO_2 h^{-1}. The pilot includes a pre-treatment unit to cool down the gas and remove impurities (SO_x, NO_x), water, and dust. The capture unit is based on Vacuum-Temperature Swing Adsorption (VTSA) technology, comprising three parallel adsorption columns operating in cyclic adsorption–desorption modes.
An extensive laboratory-scale experimental campaign was conducted prior to pilot operation. Zeolite 13X was selected as the sorbent material and formulated into a suspension to coat honeycomb structures with a thin sorbent layer. The normalised CO_2 adsorption isotherm capacity was comparable to that of the virgin powder (Figure 1a), while a significant reduction in pressure drop with respect to zeolite beads was achieved (Figure 1b). Dynamic breakthrough experiments were performed to investigate adsorption kinetics for different honeycombs, and a mathematical model was developed to extract key mass-transfer coefficients (Figure 1c). The laboratory-scale results provide an essential input for the development of a robust process model to guide pilot plant operation.

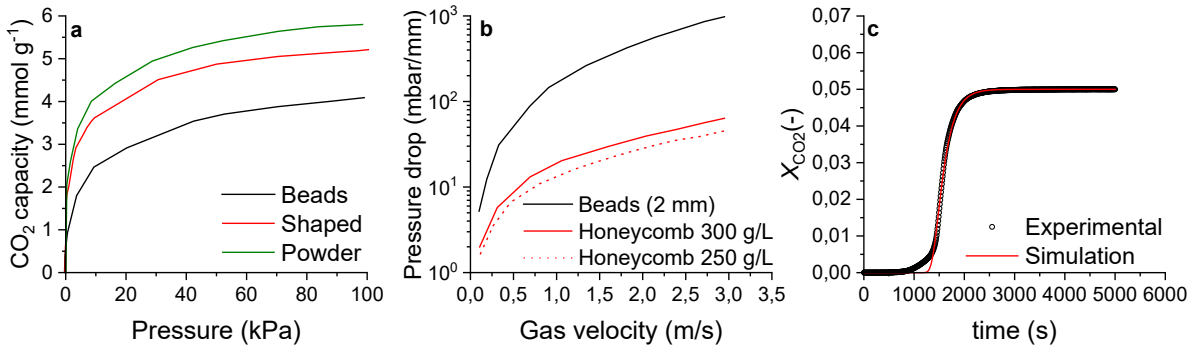

Fig. 3. a) isotherm capacities b) pressure drop measurements and c) dynamic breakthrough experiments.

Acknowledgements: The work was conducted within the Carbon4Minerals project (https://www.carbon4minerals.eu) funded by the European Union's Framework Programme for Research and Innovation Horizon Europe under Grant Agreement No. 101091870.

EES - D1 - P20
Development of 3D-printed composites of PLA reinforced with biomass

Regina Silva[1], Faozia Tayari[1], Rui Ribeiro[2], Pedro Pinto[2], Isabel Cardoso[2], Tiago Brilhante[2], Artur Ferreira[1], Vânia Teixeira[3], Nuno Gama[1]
[1]CICECO – Aveiro Institute of Materials and University of Aveiro, Portugal; [2]Amplitude Acoustics – Acústica e Vibração, Lda., Portugal; [3]Lightenjin Iluminação, Portugal

In this study, new composites based on poly(lactic acid) (PLA) and renewable raw materials (cork, rice husk, coffee grounds and oak gall with loadings ranging from 2.5% to 20.0% ($w.w^{-1}$)) were developed [1]. PLA-biomass composites were then extruded and subsequently used for 3D printing [2], having the results showed that the addition of biomass reduced the mechanical performance of the composites, as commonly observed in lignocellulosic-filled PLA systems [3]. This was particularly evident in the case of oak gall, although the properties remained adequate for 3D printing. Furthermore, the incorporation of rice husk and coffee grounds increased the filament density, whereas cork and oak gall decreased it. Regarding the thermal properties, the glass transition temperatures (T_g) of all materials remained close to 70 °C, consistent with typical PLA behaviour [4], while the thermal stability of the composites exceeded the processing temperature, indicating that the presence of biomass did not significantly compromise thermal resistance. The sustainable composites demonstrated that the coffee grounds composites demonstrated the greatest tendency toward porosity, whereas cork and rice husk promoted more uniform deposition. Despite the variability introduced by the different fillers, all formulations maintained adequate interlayer adhesion, confirming their suitability for fused-filament 3D printing. Overall, the results suggest that incorporating these bio-based raw materials into PLA is a promising strategy for developing more environmentally friendly composites.

Funding: This research was funded by FEDER – Fundo Europeu de Desenvolvimento Regional funds through of Programa Inovação e Transição Digital in the scope of the project “BiMAIS”, COMPETE2030-FEDER-01195100, and was developed within the scope of the project CICECO – Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

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EES - D1 - P21

Combining microwave-induced CO_2 plasma with a carbon bed: optimizing conversion and energy cost

Hugo Vallet[1,2,3], Omar Biondo[1,2,3], Christian K. Kiefer[1,2,3], Yury Gorbanev[1,2,3], Annemie Bogaerts[1,2,3]
[1]*PLASMANT, Dept. of Chemistry, University of Antwerp, Belgium;* [2]*Electrification Institute, University of Antwerp, Belgium;* [3]*Center of Excellence PLASMA, University of Antwerp, Belgium*

In recent years, studies on microwave-induced CO_2 plasma splitting have reported conversion values of up to 50% [1]. However, such performance is generally achieved only at low pressures (≤ 200 mbar), which presents an unfavourable operating condition for industrial application. Therefore, current research aims to maximize conversion under atmospheric conditions – which is mainly limited by recombination reactions in the plasma effluent – while also minimizing the energy cost. Recent studies have shown that rapid gas quenching enhances performance, yielding results similar to – and even exceeding – those obtained at low pressure [2, 3]. However, rapid gas quenching methods do not utilize the energy extracted from the plasma effluent. To address this, we have added a carbon bed post-plasma, which utilizes the residual energy of the plasma effluent to drive the endothermic reverse Boudouard reaction between CO_2 and C, thereby further enhancing CO formation and thus increasing conversion [4]. In addition, the carbon bed acts as an oxygen scavenger, enabling oxygen separation from the exhaust gas mixture, which is highly relevant for industry. In this research, we developed two different carbon bed designs, and we performed experiments at atmospheric pressure using a 2.45 GHz microwave reactor, with a maximum output power of 6 kW. We varied the deposited plasma power and gas flow rate to investigate their effect on the CO_2 conversion and energy cost. The results obtained show CO_2 conversion up to 73%, which is beyond the state of the art, while achieving competitive results for the energy cost, of 0.44 MJ/mol or 2.78 kWh/kg_{CO2}, thus establishing a foundation for subsequent pilot-scale implementation.

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EES - D1 - P22

First-principles insights into CO_2 reduction and the competing HER on transition metal-loaded $Zr_{12}O_{12}$ nanocages

Sajjad Hussain[1,2], Abdulaziz A. Al-Saadi[1,2,*]
[1]Dept. of Chemistry, King Fahd University of Petroleum & Minerals, Saudi Arabia; [2]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia
*Corresponding author: asaadi@kfupm.edu.sa

The catalytic reduction of CO_2 into value-added chemicals using renewable energy is a promising strategy for effective CO_2 management. However, the competing hydrogen evolution reaction (HER) significantly hinders the reaction's efficiency and product selectivity. Herein, $Zr_{12}O_{12}$ and $M@Zr_{12}O_{12}$ (M = Fe, Co, Ni, Cu, Zn) nanocages have been investigated for the photocatalytic CO_2 reduction reaction (CO_2RR) using first-principles calculations. It was observed that Fe, Co, and Ni atoms are stable on the $Zr_{12}O_{12}$ nanocages, whereas Cu and Zn atoms are not stabilized due to the lack of suitable active sites on the nanocage. Electronic structure calculations reveal that the band gap of pristine $Zr_{12}O_{12}$ is significantly reduced to 2.07 eV, which is further decreased upon loading with Fe, Co, and Ni. Notably, pristine $Zr_{12}O_{12}$ can convert CO_2 to CO under a relatively low potential of 0.71 eV. However, the desorption of CO from $Fe@Zr_{12}O_{12}$, $Co@Zr_{12}O_{12}$, and $Ni@Zr_{12}O_{12}$ nanocages is thermodynamically unfavorable due to large energy barriers. Interestingly, the $Ni@Zr_{12}O_{12}$ nanocage can spontaneously reduce CO_2 to OCCO, an important intermediate in the formation of C_2 products. But unfortunately, the strong binding energy of H atom on $Ni@Zr_{12}O_{12}$ may block active sites, thereby hindering the CO_2RR. In contrast, $Zr_{12}O_{12}$, $Fe@Zr_{12}O_{12}$, and $Co@Zr_{12}O_{12}$ can form OCCO intermediates under external energies of 0.71, 0.67, and 0.69 eV, respectively. Moreover, $Fe@Zr_{12}O_{12}$ and $Co@Zr_{12}O_{12}$ nanocages exhibit stronger CO_2 adsorption than H adsorption, which may favor the CO_2 reduction reaction.

Keywords: Zr12O12 nanocage; single-atom catalyst; CO desorption; C-C coupling.

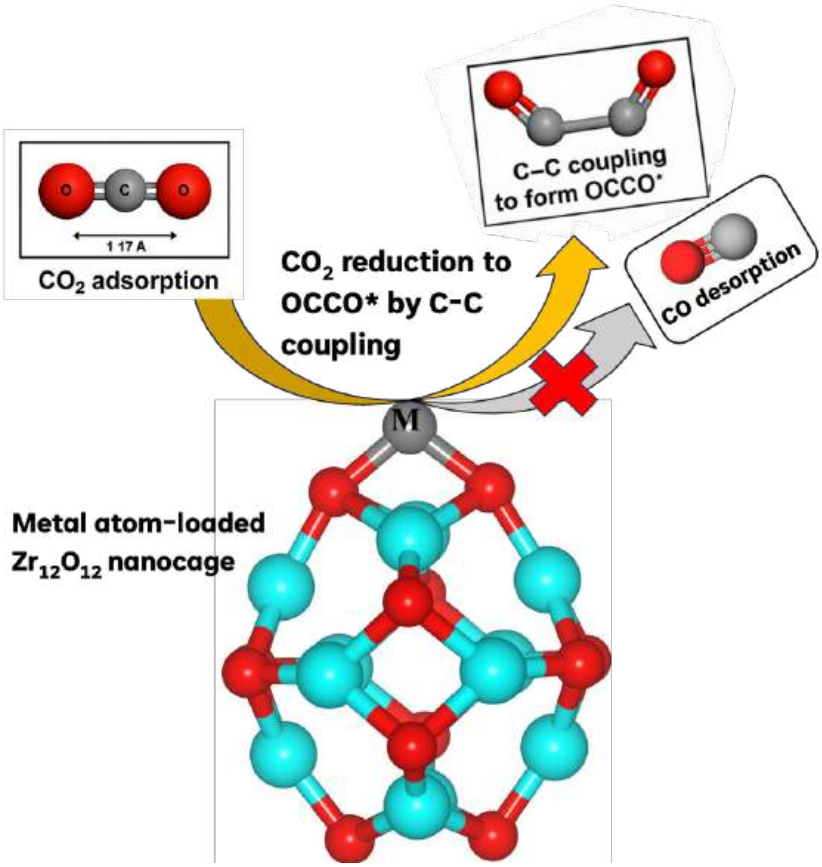

Fig. 1. C–C coupling reaction on the metal-loaded $Zr_{12}O_{12}$ nanocage.

EES - D1 - P23

Rapid mechanosynthesis of carbon-doped nickel sulfides for efficient evolution of hydrogen via water splitting

Imelda Octa Tampubolon[1,2], Róbert Džunda[3], Magdaléna Strečková[3], Matej Baláž[1]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia; [2]Faculty of Materials, Metallurgy and Recycling, Technical University of Košice, Slovakia; [3]Institute of Materials Research, Slovak Academy of Sciences, Slovakia

Global warming has intensified over recent decades, driving the transition from fossil fuels to green energy sources. Hydrogen emerges as a promising alternative, producible via water splitting.[1] Nickel sulfides, as cost-effective, conductive, and stable substitutes for platinum, have attracted significant attention for the electrocatalytic hydrogen evolution reaction (HER).[2] Doping with carbon can further improve their HER performance.[3] In this study, we synthesized a series of carbon-doped nickel sulfides with varying carbon content (0-0.4 mmol) using a mechanically-induced self-propagating reaction.[4] In this way, β-$NiS_{0.997}$, α-Ni_7S_6, and Ni_3S_2 was produced. The reaction was completed in about ten seconds. Increasing carbon content shifted the phase composition, decreasing the intensity of α-Ni_7S_6 while enhancing that of β-$NiS_{0.997}$ within seconds. The products are composed of micrometer-sized agglomerates, as confirmed by the SEM images. The electrochemical tests showed that double-layer capacitance (C_{dl}), assumed to be proportional to electrochemically active surface area, increased from 2.35 μF.cm^{-2} to 10.61 μF.cm^{-2} as the carbon content increased from 0 to 0.4 mmol. The electrocatalytic performance was also significantly improved, with the overpotential dropping from 254 mV (undoped NiS) to 191 mV when doping with 0.4 mmol carbon, revealing a direct correlation between carbon doping and HER efficiency.

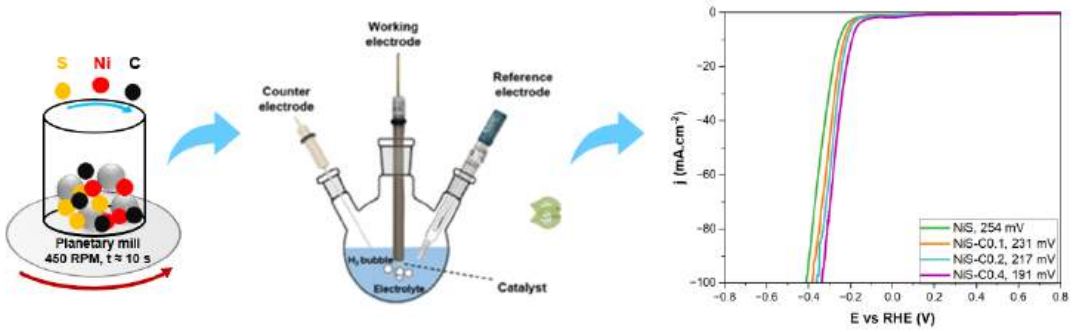

Fig. 1. Synthesis and electrocatalytic performance of nickel sulfide electrocatalysts

This work was supported by the Slovak Research and Development Agency (contract no. APVV-24-0353).

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EES - D1 - P25
Silica coating of PEM fuel cell Pt/carbon electrocatalysts to enhance durability upon operation

Lucas Elvira[1], Ali Haider[1,2], Loïc Noumbi[2], Nathalie Job[2], Sophie Hermans[1]
[1]IMCN Institute (MOST division), UCLouvain, Belgium; [2]Nanomaterials, Catalysis, Electrochemistry (NCE), University of Liège, Belgium

Proton Exchange Membrane Fuel Cells (PEMFCs) are promising electrochemical devices for the production of zero-emission electricity. Platinum supported on carbon black (Pt/CB) is the primary catalyst used in practical PEMFC applications due to its high activity but the harsh operating conditions accelerate the catalyst degradation, compromising stability and long-term fuel cell efficiency[1].
As a potential solution, silica-coating methods have been reported in the literature to improve catalyst stability[2,3]. A porous silica layer can act as a protective barrier, limiting particle dissolution and sintering while maintaining access for the reactants to the Pt particles. As catalysts support, Carbon Xerogels (CXs) are promising candidates due to their tunable meso/macroporosity, which allows optimization of mass transport properties[4].
This project aims to develop silica-coating methods for Pt/CX catalysts, with a focus on achieving controlled layer thickness, uniform coatings and pores structure, through statistical analysis and optimization of synthesis parameters. The catalysts are characterized using physicochemical techniques (Fig. 1) as well as electrochemical measurements on Rotating Disk Electrode systems. Ultimately, the most promising catalysts will be integrated into a membrane-electrode assembly (MEA) for performance evaluation.

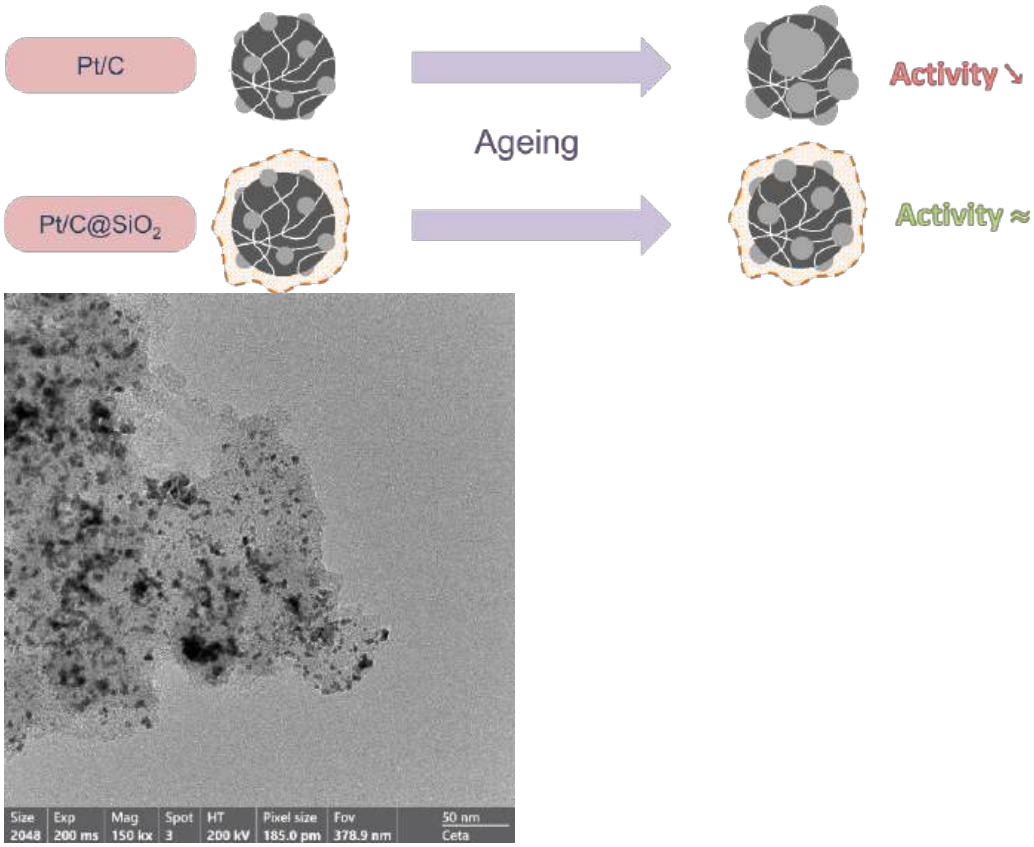

Fig. 1. (up) Goal of the project and (bottom) TEM image of a Pt/CX sample covered by a silica layer

The authors thank the F.R.S-FNRS for providing funding via a PDR project (Convention T.0166.24) and would like to acknowledge the financial support from the Walloon Region Win4Excellence project “TiNTHyN” under contract n°2310142, granted by SPW-Economie Emploi Recherche and supported by the Plan de Relance de la Wallonie.

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EES - D1 - P26

Improved chemical recycling of PET derivatives: Enhanced glycolysis via morphology control and catalysis

Chang joon Park[1], Geon kyo Park[1], Hyun Min Jung[1]*
[1]Dept. of Applied Chemistry, Kumoh National Institute of Technology, Republic of Korea

Polyethylene terephthalate (PET) and its derivatives, such as poly(1,4-cyclohexylenedimethylene terephthalate) (PCT), are widely used in fibers, films, and packaging due to their excellent chemical resistance, durability, and transparency. However, their extensive use has led to growing concerns about plastic waste. Chemical recycling methods, such as glycolysis, have emerged as effective solutions, converting waste plastics into valuable monomers. Typically, ethylene glycol (EG) is used to degrade PET into bis(2-hydroxyethyl) terephthalate (BHET), a monomer that can be reused for PET production. Diols like diethylene glycol (DEG), cyclohexanedimethanol (CHDM), and d-isosorbide (ISB) are also utilized to diversify the glycolysis products. Despite this, the effect of these diols on glycolysis rates has not been fully explored. Our study investigates the impact of various diols on the glycolysis efficiency of PET and PCT, revealing that steric hindrance due to the bulky diol structures significantly impairs reaction rates. For instance, PET glycolysis with ISB shows a remarkably low reaction rate of 0.17%, whereas DEG and CHDM result in rates approximately 0.28% of those observed for PET. Additionally, the rigid structure of PCT leads to a glycolysis efficiency with DEG that is only one-third of that of PET. To address these challenges, we propose an enhanced glycolysis process using morphology control and advanced catalysts. Pre-treatment of PET with dimethyl sulfoxide (DMSO) improves its structure, increasing glycolysis rates at lower temperatures. For PCT and PIT, a novel catalyst combination of zinc ions and alkoxy species was tested, yielding a threefold improvement in conversion compared to conventional zinc catalysts. Under optimized conditions, PET was successfully converted into low-molecular-weight polyols, demonstrating the potential for direct applications in rigid polyurethane production. This work presents significant advances in enhancing glycolysis for PET derivatives, paving the way for efficient chemical recycling at lower temperatures.

EES - D1 - P27
Co-doped $BiVO_4$ isotype homojunctions for enhanced photocatalytic water treatment

Tayebeh Sharifi[1], Tecush Mohammadi[2], Marko Štrok[1]
[1]Jožef Stefan Institute, Slovenia; [2]National Institute of Chemistry, Slovenia

Harnessing solar energy through semiconductor-based photocatalysis, particularly visible light active materials, represents a sustainable and versatile approach for addressing global challenges related to energy conversion and environmental remediation. Among them, $BiVO_4$ has attracted considerable attention for a variety of photocatalytic applications due to its appropriate band gap (~2.4 eV), chemical stability, and low toxicity. Nevertheless, its practical performance remains constrained by intrinsic limitations (e.g., short charge-carrier diffusion lengths and severe photogenerated e-/h+ recombination).To mitigate these drawbacks, extensive efforts have been dedicated including (non)metal doping, heterojunction formation, and isotype homojunction engineering. In particular, isotype homojunctions within $BiVO_4$ have recently emerged as an effective means to facilitate charge separation. In parallel, transition-metal doping has been shown to introduce controlled defect states and modulate band structure, offering an additional handle to enhance charge transport properties.
In this work, co-precipitation route was employed to synthesize isotype homojunction $BiVO_4$, followed by cobalt (Co) incorporation. The combined effects of phase junction formation and Co doping were systematically investigated, with the aim of improving charge separation and transportion efficiency. The photoactivity of the materials was evaluated using photocurrent measurement. Charge-transfer processes were also analyzed using electrochemical impedance spectroscopy under dark and illuminated conditions. Moreover, methyl orange was employed as a representative organic pollutant to assess photocatalytic degradation performance under light irradiation. The results demonstrate that Co-doped isotype homojunction $BiVO_4$ exhibits enhanced photocatalytic and photoelectrochemical activity, highlighting the synergistic role of homojunction engineering and dopant-induced electronic modulation for water treatment and solar energy conversion applications.

Acknowledgements: This research was funded by the European Union under the HORIZON-MSCA-2021-PF-01 program (BPEC-DW project, GA No. 101061873) and Slovenian Research and Innovation Agency (Projects N1-0401).

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EES - D1 - P28
Slurry electrolysis for sustainable copper recovery from electronic waste

Adriana Vulcu[1], Camelia Berghian-Grosan[1], Angela Kasza[1], Gabriel Katona[2]
[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Romania; [2]Babes-Bolyai University, Romania

The rapid expansion of industrial activities contributes to a substantial increase in waste generation, particularly electrical and electronic waste (e-waste). This waste stream is characterized by high concentrations of metals and hazardous substances, making it a significant source of emerging environmental pollutants. E-waste represents a valuable secondary resource, containing important amounts of precious and non-precious metals, such as gold, silver, and copper. Among these, copper is the most abundant, accounting for approximately 20–55% of the total metal content in e-waste, which makes its recovery particularly important. Electrolytic copper recovery methods offer distinct advantages over conventional technologies, including high selectivity and product purity, as well as operation under mild conditions, such as ambient temperature and atmospheric pressure. In this work, we investigated the influence of the anode nature on the recovery of copper from waste printed circuit boards (WPCBs) using slurry electrolysis. Before the electrochemical recovery, the WCPBs were mechanically and chemically pre-treated. The copper electrolysis was performed in a custom-built electrolyzer equipped with an anode and a copper cathode, using the H_2SO_4–$CuSO_4$–NaCl system as electrolyte and an in-house DC power supply, at room temperature. Several anodes, such as stainless steel, titanium, and graphite, were tested in order to obtain the best copper conversion efficiency and purity. Also, the influence of key operating parameters, including WPCB scraps concentration, current density, electrolyte composition, and electrolysis time, was examined to evaluate copper recovery efficiency and selectivity. The best results were obtained using a graphite anode with a copper conversion efficiency of approximately 70%, with the recovered copper exhibiting a purity of about 85%. The technology is demonstrated at a lab scale. The findings provide a basis for further optimization and scale-up of electrochemical recycling processes for complex waste streams.

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0095, within PNCDI IV.

EES - D1 - P29
Direct electrochemical processing of e-waste for sustainable copper recovery

Camelia Berghian-Grosan[1], Adriana Vulcu[1], Angela Kasza[1], Gabriel Katona[2]
[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Romania; [2]Babes-Bolyai University, Romania

The rising amounts of electronic waste, including waste printed circuit boards (WPCBs), contribute to serious environmental challenges but also represent an important secondary resource for critical and non-precious metals, notably copper. The development of sustainable and efficient recovery technologies is therefore essential. In this work, we investigated a direct electrolysis approach for copper recovery from WPCBs to enable a simplified and greener recycling route. Copper-rich WPCBs fractions, obtained after mechanical pretreatment, were directly subjected to electrochemical processing without extensive chemical leaching or purification steps. The process consists of the anodic dissolution of copper from the solid waste matrix and its subsequent cathodic electrodeposition as metallic copper. Metal scrap powder obtained from WPCBs was compacted by hydraulic pressing to form plate-shaped anodes. The electrolysis process was performed in a custom-built electrolyzer equipped with a solid anode and a copper cathode, using the H_2SO_4–$CuSO_4$–NaCl system as electrolyte and an in-house DC power supply. The influence of electrochemical parameters, including current density, electrolyte composition, and electrolysis duration, was investigated to optimize copper recovery efficiency and selectivity. The deposited copper was structurally and morphologically characterized. The preliminary results indicate a conversion efficiency of ~52% and a recovered copper purity of 72%, demonstrating effective copper recovery with limited interference from co-existing metals typically present in the WPCBs. From an environmental perspective, the direct electrolysis strategy reduces reagent consumption, minimizes secondary waste generation, and shortens process flows compared to conventional hydrometallurgical and pyrometallurgical routes.

This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0095, within PNCDI IV.

EES - D1 - P30

Antiviral Co-doped ZnO pigments: Solution combustion synthesis using *Aloe Vera* extract as an alternative green fuel

Julia de Oliveira Primo[1], Nayara Balaba[1], Polona Umek[2], Rob Onderwater[3], Carla Bittencourt[1]
[1]University of Mons, Belgium; [2]Jožef Stefan Institute, Slovenia; [3]Materia Nova ASBL, Belgium

The use of plants as fuel in solution combustion synthesis (SCS) is a simple, low-cost method for material synthesis.1 As renewable and easily accessible resources, plants enhance the sustainability of this synthetic process.1 In this study, Aloe vera extract was evaluated as an alternative green fuel in the synthesis of inorganic pigments. The main objective was to synthesize zinc oxide (ZnO) and cobalt-doped zinc oxides (Co-ZnO) via SCS at 750 °C, using varying concentrations, for use as antiviral pigments in architectural coatings (Figure 1a).

To characterize the pigments, analyses were performed using XRD, XPS, and colorimetry (CIEL*a*b* method). The XRD profiles indicated that the obtained oxides were predominantly wurtzite, with a second phase, the spinel phase of $ZnCo_2O_4$ (Figure 1b). Raman data corroborated this result. XPS confirms the presence of Co (III) in ZnO pigments with 5% and 10% Co doping. In antiviral property studies, the pigment particles were dispersed at 10% (w/w) in a water-based acrylic binder. Coatings were applied to polycarbonate (PC) plates, and RT-PCR was used to assess SARS-CoV-2 inactivation after exposing the coated surfaces to the virus, in accordance with the adapted ISO 22196:2011 standard. The coatings were characterized using SEM/EDS, and their wettability was evaluated. The results showed that the pigments obtained by SCS exhibited clustered distribution on the surface of the coatings when dispersed in acrylic binder (Figure 1c). Wettability tests indicated that hydrophilic surfaces formed upon pigment addition to binder (CA < 90°) (Figure 1d). According to RT-PCR results, all pigments exhibited antiviral activity, with the coating surface achieving over 80% inactivation of SARS-CoV-2 after 24 hours, and inactivation increased with increasing dopant ion concentration (Table 1), compared with the reference control (PC).

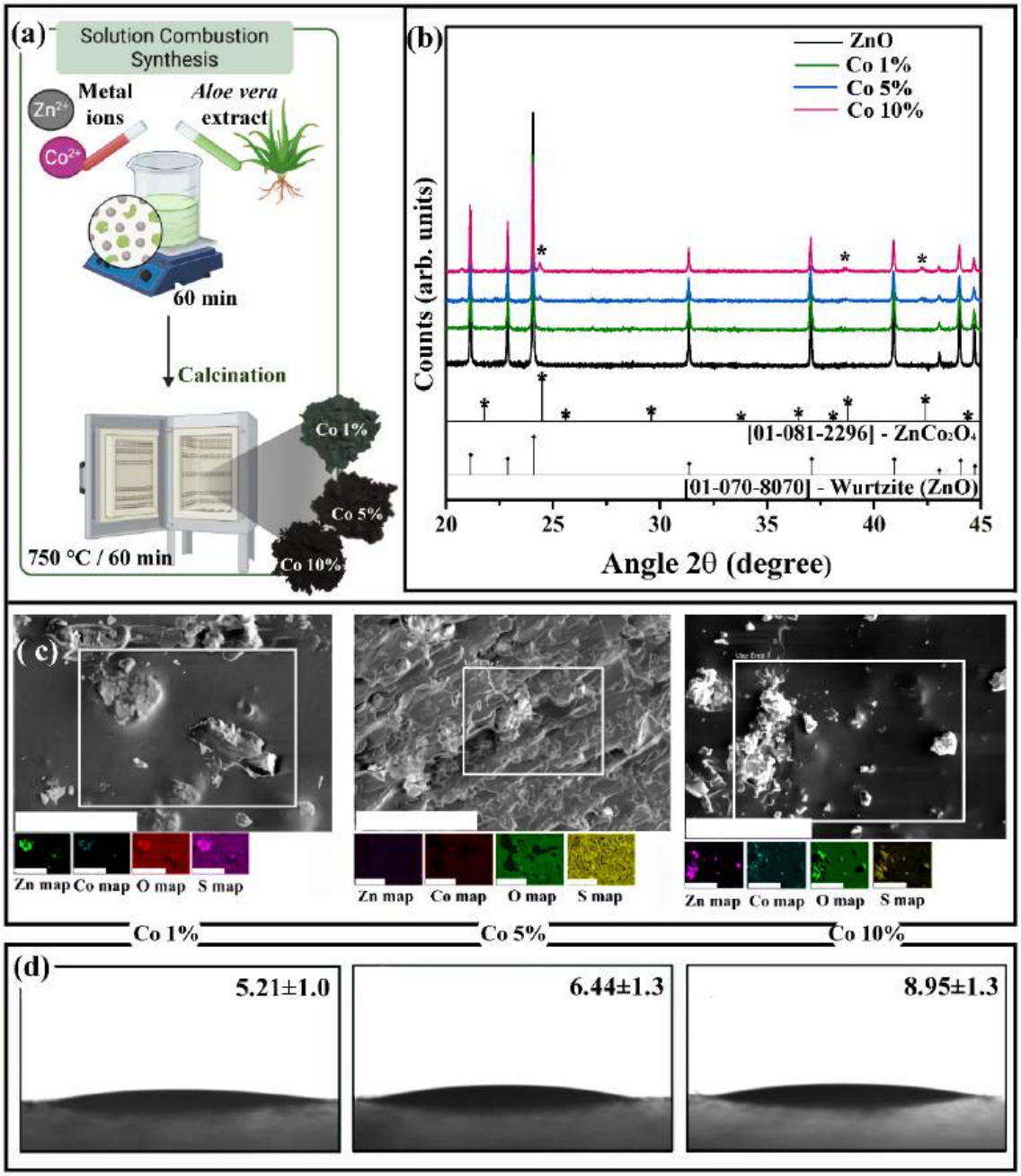

Fig. 4. (a) Schema of the SCS utilized in this study at 750 °C, with varying concentrations of the dopant ion (1%, 5%, and 10% by mass relative to Zn ions); (b) X-ray Diffraction (XRD) patterns of the synthesized pigments, with the spinel phase of $ZnCo_2O_4$ indicated by an asterisk (*) in the image; (c) Scanning Electron Microscope (SEM) mapping of the coating surface containing the pigments (Co-doped ZnO) dispersed in an acrylic binder; (d) Images of the contact angle measurements of the surfaces of Co-ZnO coatings dispersed in an acrylic binder matrix.

Sample	Ct	Reduction (%)
Policarbonate (PC)	25	0
Binder	25.5	17.7
ZnO undoped	28	80.9
Co1%	28.5	86.2
Co 5%	29.4	91.5
Co10%	29.5	97.3

Table 2. Reduction in viral load on the coating containing synthesized pigments and the control after 24 hours of exposure, as determined by RT-PCR.

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EES - D1 - P31
Sustainable chitin carbons from *Hermetia illucens* pupal waste for ethylparaben removal

Aleksandra Bazan-Wozniak[1], Sebastian Grzyb[2], Agnieszka Nosal-Wiercińska[3], Robert Pietrzak[1]
[1]Dept. of Applied Chemistry, Faculty of Chemistry, Adam Mickiewicz University in Poznań, Poland; [2]College of Engineering and Health in Warsaw, Poland; [3]Dept. of Analytical Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Sklodowska University, Poland

This study describes the preparation of activated carbons with a highly developed specific surface area, designed for efficient adsorption of ethylparaben from water. The carbons were synthesized from empty pupal shells of *Hermetia illucens*, providing a sustainable and inexpensive precursor. Chemical activation with sodium carbonate produced materials with surface areas near 1900 m^2/g, indicating a significant degree of porosity. Structural analysis showed that the obtained adsorbents contained a combination of micro- and mesopores, which promotes uptake of organic molecules through rapid diffusion and strong interactions with the surface.
Adsorption performance was evaluated using statistical physical models. The maximum adsorption capacity reached 715 mg/g, and the process followed pseudo-second-order kinetics and the Langmuir isotherm, suggesting chemisorption on a homogeneous surface with monolayer coverage. The adsorption mechanism involved several types of interactions. π-π stacking between aromatic rings, hydrogen bonding, and electrostatic attractions between ethylparaben molecules and functional groups on the carbon surface contributed to the overall performance. Thermodynamic analysis revealed that adsorption was spontaneous and endothermic, indicating that higher temperatures favor the process. Reusability tests confirmed that the materials maintained a high level of performance. After three adsorption–desorption cycles, approximately 80% desorption efficiency was retained, demonstrating that the activated carbons were stable and suitable for repeated application without major loss of capacity.
The results highlight the suitability of waste-derived biological materials as sources for producing high-quality activated carbons. Using pupal shells of *Hermetia illucens* offers an environmentally friendly and cost-effective route for preparing adsorbents with excellent performance.

EES - D1 - P32
Influence of the grinding conditions on the particle size of foam powder

Emanuele Bassani[1], Letícia D. Costa[1], Cátia Alves[1], Afonso Bangui[2], Miguel A. Pacheco[2], Lidia Gonçalves[2], Alfredo Castro[2], Miguel Pacheco[2], Artur Ferreira[1], Nuno Gama[1]
[1]CICECO – Aveiro Institute of Materials and Materials and University of Aveiro, Portugal; [2]Heliotextil, S. A. São João da Madeira, Portugal

Polyurethanes (PU) represent one of the most versatile and widely used classes of polymers, with an expected market growth of *ca.* 8% from 2025 to 2030.[1] Noteworthy, it is important to highlight that polyurethane foams (PUFs) account for about 67% of all PUs produced.[2]
However, due to their low biodegradability, their end-of-life poses significant environmental challenges, with PUF waste being mostly sent to landfill or incinerated—options that are not environmentally viable. Therefore, PU waste must be recycled, although this is particularly challenging due to their thermoset nature.[2,3] Nonetheless, mechanical recycling, which is based on shredding and grinding, is a cost-effective method that allows the conversion of PUF waste into powders with particle sizes suitable for its reuse in several applications.[3]
Following our interest in addressing the sustainability of plastics, this project focuses on the mechanical recycling of PUF waste. Given the importance of powder particles size on further applications, this study aimed to investigate the influence of the grinding conditions on the resulting powders, in order to optimize the operating conditions and meet the requirements of the target application.

This work was funded by FEDER - Fundo Europeu de Desenvolvimento Regional funds through of Programa Inovação e Transição Digital in the scope of the project “CIRATEX – Circularidade aplicada a adesivos têxteis”, COMPETE2030-FEDER-01159700, and was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

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EES - D1 - P33

Carbon adsorbents from fennel and caraway seeds via chemical activation for dexketoprofen removal

Dorota Paluch[1], Robert Wolski[1], Aleksandra Bazan-Wozniak[1], Robert Pietrzak[1]
[1]Dept. of Applied Chemistry, Faculty of Chemistry, Adam Mickiewicz University in Poznań, Poland

The increasing pressure to protect the environment has intensified the search for modern, effective and economical water treatment methods. Of the available techniques, adsorption is widely regarded as one of the most efficient ways of removing trace organic contaminants from water. Its increasing popularity is due to its straightforward operation, low running costs, and its ability to eliminate harmful substances at very low concentrations. A particularly important material in adsorption processes is activated carbon, produced from carbon-rich biomass via pyrolysis in an environment with limited oxygen. Its widespread application stems from its low production costs, minimal contribution to carbon dioxide emissions and the possibility of utilising various plant-based resources, including herbal and agricultural waste materials[1].

Activated carbon exhibits excellent adsorption performance due to its highly porous structure, large specific surface area, and favourable surface chemistry. These properties enable effective interactions between the adsorbent and pollutants dissolved in aqueous solutions. Consequently, activated carbon is widely regarded as a versatile and reliable material for water purification technologies aimed at removing organic contaminants from aqueous systems.

This study aimed to produce activated carbons by chemically activating fennel (*Foeniculum vulgare*) and caraway (*Carum carvi*) seeds using potassium carbonate and conventional heating. Their physicochemical characteristics were analysed, and their sorption properties were systematically evaluated. The resulting carbon materials were used as adsorbents to remove dexketoprofen from aqueous solutions. The obtained materials exhibited sorption capacities of 294–322 mg/g. To describe the adsorption behaviour and identify the underlying mechanisms, Langmuir and Freundlich isotherm models were applied. The effect of contact time between the adsorbent and the adsorbate was also examined in order to determine the progression of adsorption and equilibrium conditions.

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EES - D1 - P34

Supporting environmental remediation through the NanoEnviCZ infrastructure: Development of cyclodextrin-modified nanofibrous membranes

Radka Guldanová[1], Jana Štěpánová[1], Martin Stuchlík[1], Jana Müllerová, Christopher J. Hobbs[1], Michal Řezanka[1]

[1]Dept. of Nanochemistry, Technical University of Liberec, Czech Republic

By providing a comprehensive platform for the characterization of advanced nanomaterials, the NanoEnviCZ infrastructure enables the effective implementation of basic chemical research into viable technologies for remediation purposes such as water treatment.

A prime example of this synergy is the development of innovative cyclodextrin (CD)-based polymers and their incorporation onto nanofibrous membranes. By utilizing the natural, biodegradable properties and unique truncated cone structure of these CDs, we create materials capable of forming host-guest inclusion complexes with various organic pollutants. This approach combines the specific molecular recognition of CD polymers with the high surface-to-volume ratio of nanofibers to effectively absorb emerging contaminants.

Using the array of available advanced instrumentation of the NanoEnviCZ infrastructure, we have characterized these functionalized nanomaterials and demonstrated their high removal efficiency toward pollutants in laboratory-scale aqueous solutions. Our research evaluates the removal of a broad range of contaminants, including pesticides and pharmaceuticals[1,2], with a shifting emphasis toward the effective capture of per- and polyfluoroalkyl substances (PFAS). These findings not only demonstrate the potential of cyclodextrin-modified membranes as a sustainable basis for future water treatment but also underscores the crucial role of specialized research infrastructures, like NanoEnviCz, in fostering the development of advanced bio-based technologies for environmental protection.

Acknowledgement: The authors acknowledge the assistance provided by the Research Infrastructure NanoEnviCZ, supported by the Ministry of Education, Youth, and Sports of the Czech Republic under Project No. LM2023066.

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EES - D1 - P35

Establishing Raman spectral references for climate- and energy-relevant materials through ab initio dynamics and experimental tools

Fileto Rodríguez[1], Jianing Wang[1], Ionut Tranca[1], Enrique Lozano[2], Mónica Calatayud[3], Frederik Tielens[1]
[1]Vrije University Brussel, Belgium; [2]ELODIZ Ltd., UK; [3]Sorbonne Université, France

Establishing precise reference data that enables the use of green characterization techniques is essential for advancing sustainable materials science. In this context, theoretical spectroscopy has demonstrated strong capabilities, with dynamic Raman spectroscopy offering a powerful computational framework to account for physical effects, such as anharmonicity and finite temperature, that strongly influence vibrational responses but are often neglected in conventional Raman simulations. Although these effects are crucial for realistic materials characterization, their inclusion in periodic systems remains challenging, limiting the applicability of dynamic Raman to solid-state materials. In this work, we broaden the applicability of dynamic Raman spectroscopy by extending Voronoi radical tessellation to molecular ionic solids.[1]

We introduce a fully *ab initio* protocol in which tessellation parameters are derived from Bader's quantum theory of atoms in molecules (QTAIM), avoiding the need for empirical input. The accuracy and robustness of the approach are validated through direct comparison of computed vibrational spectra with experimental data and distinct computational approaches.[2]

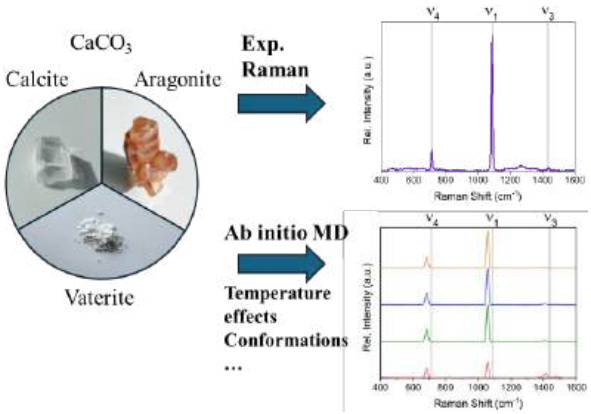
The versatility and relevance of the method are demonstrated through applications to three classes of materials, selected for their connection to climate and energy challenges:

(i) Calcium carbonates, key biominerals in several biological processes and geochemical carbon cycling.

(ii) Solid electrolytes, central to the development of safer and more sustainable all-solid-state batteries.

(iii) Low cobalt content cathode active materials, essential for reducing reliance on critical raw materials in energy-storage technologies.

By providing reliable Raman references for these materials, our work supports the broader adoption of Raman spectroscopy as a fast, non-destructive, and environmentally friendly characterization tool. This approach enables more sustainable characterization protocols for both academic research and industrial development, contributing to ongoing efforts to address climate and energy challenges.



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EES - D1 - P36
Insights into electro-oxidative dehydrogenation of aldehydes on copper foam

Benni. Zou[1], Sonja D. Mürtz[1], Regina Palkovits[1,2,3]
[1]Institute for Technical and Macromolecular Chemistry (ITMC), RWTH Aachen University, Germany; [2]Institute for a Sustainable Hydrogen Economy (INW-2) Forschungszentrum Jülich GmbH, Germany; [3]Max-Planck-Institute for Chemical Energy Conversion, Germany

The high energy demand of the oxygen evolution reaction constitutes a major bottleneck for green hydrogen production via water electrolysis. Biomass-derived aldehyde electrooxidative dehydrogenation (EOD), which can operate at low potentials, provides an effective alternative anodic pathway to reduce the overall cell voltage. Representative biomass aldehydes such as furfural can be selectively converted at the anode into high-value furoic acid while simultaneously releasing half an equivalent of green hydrogen, thereby offering both improved energy efficiency and chemical valorization. However, a systematic understanding of the catalyst structure-performance relationships and the competitive interplay between Faradaic and non-Faradaic processes in these reactions remains lacking.
In this study, furfural was employed as a model substrate to systematically investigate its electrooxidative dehydrogenation behavior on modified copper foam anodes. By tuning the wet-chemical oxidation conditions, copper foam electrodes with distinct morphologies were constructed, revealing intrinsic correlations between electrode structure, electrochemically active surface area, charge-transfer characteristics, and reaction kinetics. A stable current density of up to 110 mA cm^{-2} was achieved at 0.3 V versus the reversible hydrogen electrode (RHE). The results demonstrate that increasing substrate concentration accelerates reaction rates but significantly promotes non-Faradaic disproportionation side reactions, thereby compromising Faradaic efficiency, whereas lowering the alkaline electrolyte concentration effectively suppresses these parasitic pathways[1]. Substrate screening indicated reduced activity for aldehydes with high electron density, potentially due to inhibited intermediate formation. By systematically examining substrate structure, concentration, pH, and electrode optimization, this work delineates the operational boundaries between Faradaic and non-Faradaic molecular processes during electrolysis. Overall, this study substantially advances the mechanistic understanding of furfural electro-oxidative dehydrogenation with dual-electrode green hydrogen production.

Acknowledgements: Financial support from the Federal Ministry of Research, Technology and Space (BMFTR) within the project (ID: 03SF0727A) Hydrogen4Tomorrow is gratefully acknowledged. This work was also supported by the Cluster of Excellence Fuel Science Center (EXC 2186, ID: 390919832) funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities. The authors acknowledge the funding by the German Federal Ministry of Research, Technology and Space (BMFTR) and the Ministry of Economic Affairs, Industry, Climate Action and Energy of the State of North Rhine-Westphalia through the project HC-H2.

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EES - D1 - P37
BiOI/SnO_2 nanofibers for robust visible-light/PMS-driven multipollutant mineralization

Laura Huidobro[1,2], Jordi Rigual-Miret[1,2], Miquel Allés[3], Mahmoud Abid[4], Mikhael Bechelany[4], Carmen Sousa[3], Elvira Gómez[1,2], Albert Serrà[1,2]*
[1]Dept. de Ciència de Materials i Química Física, Universitat de Barcelona, Spain; [2]Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Spain; [3]Dept. de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Spain; [4]Institut Européen des Membranes (IEM), University of Montpellier, France

Emerging contaminants (ECs) in aquatic environments, particularly pharmaceuticals, represent a major environmental concern due to their persistence, limited biodegradability, and resistance to conventional wastewater treatment processes, contributing to the spread of antimicrobial resistance. In this context, advanced oxidation processes (AOPs), based on the generation of highly reactive oxygen species, have gained increasing attention as effective complementary strategies for water remediation.
In this work, photocatalytic BiOI/SnO_2 composite nanofibers (NFs) were developed via a one-step electrospinning process, in which BiOI microspheres were directly incorporated into the spinning solution. Comprehensive morphological, structural, and optical characterizations confirmed the successful formation of the composite nanofibers. Density functional theory (DFT) calculations, supported by XPS analysis, revealed the formation of an S-scheme SnO_2/BiOI heterojunction, promoting efficient spatial separation of photogenerated charge carriers.
Photocatalytic activity was evaluated under visible-light irradiation, and further enhanced by the addition of peroxymonosulfate (PMS), leading to the generation of highly reactive sulfate radicals, using tetracycline (TC) as target contaminant. The BiOI/SnO_2 NFs achieved over 97% TC degradation and 91% mineralization within 90 minutes. Moreover, the catalyst demonstrated high versatility and stability in multi-contaminant systems and tap water matrices, maintaining over 80% mineralization efficiency with negligible leaching and sustained performance over multiple cycles.
These findings highlight the potential of electrospun BiOI/SnO2 nanofibers as efficient, robust, and scalable photocatalysts for the removal of emerging contaminants from water, offering a promising strategy for environmental remediation.

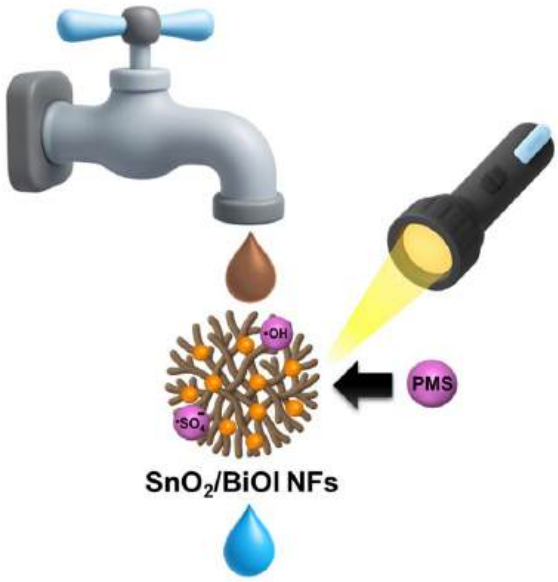

Fig. 5. Schematic illustration of visible-light/PMS-activated multipollutant degradation over electrospun SnO_2/BiOI nanofibers.

Acknowledgements: Grant CNS2024-154690 funded by MICIU/AEI/10.13039/501100011033 and, as appropriate, by “ESF Investing in your future”, by “ESF+” or by “European Union NextGenerationEU/PRTR”. The authors also would like to express their gratitude to the Departament de Recerca i Universitats, particularly the Departament d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR) for their support. Authors thank the CCiT-UB for the use of their equipment.

EES - D1 - P38

Development of hollow bimetallic catalysts supported on nanostructured carbons for sustainable PEM fuel cell electrodes

Ali Haider[1,2], Lucas Elvira[2], Loïc Noumbi[1], Sophie Hermans[2], Nathalie Job[1]
[1]University of Liège, Dept. of Chemical Engineering (B6a), Belgium; [2]UCLouvain, IMCN Institute, Belgium

Proton Exchange Membrane (PEM) fuel cells offer an efficient method to convert hydrogen and oxygen into electricity and water. The catalytic layers of a PEM fuel cell are typically composed of Pt nanoparticles (NPs, ~3 nm in size) supported on carbon black and mixed with a polymer ionomer (Nafion®)[1]. However, upon operation, both the carbon support and the Pt nanoparticles degrade[2]: carbon undergoes oxidation, while Pt particles coalesce or dissolve and redeposit elsewhere, resulting in performance decay.

To enhance catalyst efficiency and lifetime, our research has focused on developing hollow PtM nanoparticles. In particular, large (10–50 nm) hollow PtCo nanoparticles degrade more slowly[3]. Alloying Pt with transition metals such as Co or Ni contracts the Pt lattice, which reduces the binding energy of oxygen reduction intermediates[4]. In addition, as a support material, carbon xerogels (CXs) offer an interesting alternative to carbon black, as their tunable pore texture can reduce diffusion-induced voltage losses (η_{diff})[5]. The stability of CX supports can be further improved by applying a thin graphitic coating via Chemical Vapor Deposition (CVD)[6].

PtCo/CX catalysts have been synthesized in previous work[3], but the 14-step procedure is too complex and requires simplification. The main goal of this work is to rationalize and optimize the synthesis route for hollow PtCo/CX catalysts. Catalysts were prepared on CX supports with controlled mesopore size (50–100 nm) and subsequently coated with a graphitic carbon layer via CVD. The hollow PtCo/CX catalysts were characterized using physico-chemical methods (Fig.1) and evaluated electrochemically in 0.1 M $HClO_4$, exhibiting higher mass and specific activities than commercial Vulcan Pt/C material.

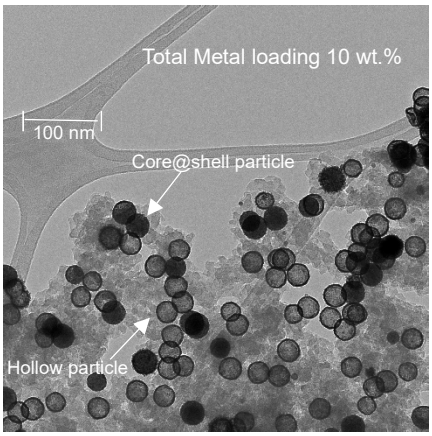

Fig. 1. TEM image of catalyst PtCo/CX

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EES - D1 - P39
Green synthesis of silver nanoparticles using plant extract for water disinfection

Arleth Gualle[1], Carla Bittencourt[1], Lourdes M. Orejuela-Escobar[2,3]
[1]Chimie des Interactions Plasma-Surface (ChIPS), Research Institute for Materials Science and Engineering, University of Mons, Belgium; [2]Universidad San Francisco de Quito USFQ, Colegio de Ciencias e Ingenierías; Applied Circular Engineering & Simulation Group (GICAS), Chemical Engineering Dept., Ecuador; [3]Geocircular Consulting Group, USA

Access to safe water is one of the most critical humanitarian challenges worldwide. It is estimated that approximately 2.2 billion people lack access to safe drinking water, a situation exacerbated by poor water management and increasing demand[1]. Conventional water treatment methods, such as chlorination and ultraviolet irradiation, are effective but may generate harmful disinfection byproducts and contribute to bacterial resistance[2]. In this context, nanomaterials have emerged as promising alternatives for water disinfection due to their high surface-to-volume ratio and unique mechanical, electrical, optical, and magnetic properties, which enable applications in catalysis, adsorption, and enhanced reactivity.[3].
Within a more eco-friendly approach to metallic nanoparticle synthesis, green synthesis (GS) has been widely explored as a sustainable alternative to conventional chemical methods[4]. Plant extracts and agro-industrial residues contain phytoactive compounds such as polyphenols, tannins, and proteins that act as both reducing and capping agents, promoting the reduction of Ag^{+} to Ag^{0} and stabilizing the resulting nanoparticles [5]. In this study, a blue LED-assisted GS method (450–460 nm) was developed for the synthesis of silver nanoparticles (AgNPs) using avocado seed extracts obtained by Soxhlet extraction with three solvents: water (AV-H), ethanol (AV-ET), and methanol (AV-MET) see Figure 1.
Surface plasmon resonance (SPR) analysis revealed enhanced AgNP formation in the aqueous extract, as indicated by a more intense and well-defined SPR band near 450 nm. SEM analysis confirmed the spherical morphology of AgNPs synthesized in AV-H_2O, which exhibited smaller particle size, improved uniformity, and reduced aggregation compared to those obtained with AV-ET and AV-MET. Additionally, pH was identified as a determining factor, as acidic conditions limit nanoparticle formation, whereas neutral to alkaline environments favor Ag^{+} reduction by enhancing the ionization and reducing capacity of phytocompounds. Overall, the green synthesis of AgNPs using aqueous extracts is environmentally friendly, cost-effective, and offers strong potential for future water treatment applications based on agro-industrial residues.

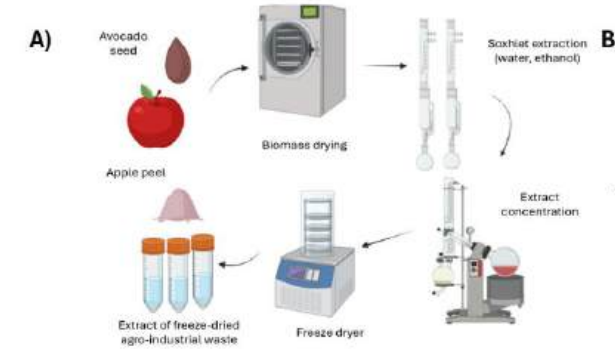

Fig 1. Process for obtaining extracts from agro-industrial residues

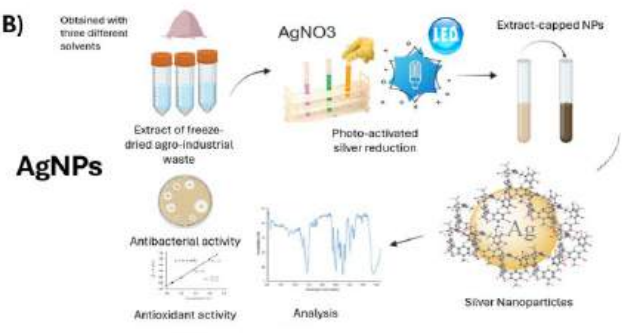

Fig 2. Synthesis of silver nanoparticles under LED light

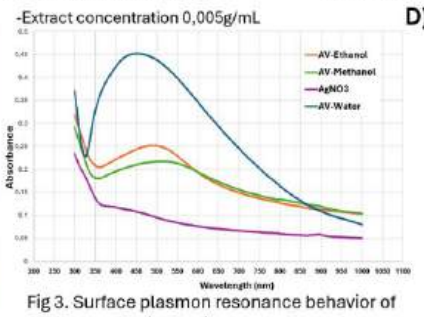

Fig 3. Surface plasmon resonance behavior of AgNPs synthesized using avocado seed extracts under green synthesis conditions

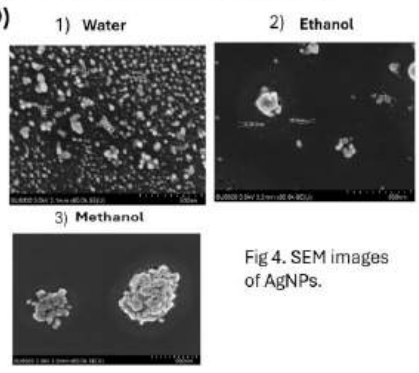

Fig 4. SEM images of AgNPs.

Fig. 1. Green synthesis and characterization of silver nanoparticles (AgNPs) using avocado seed extracts obtained with three different solvents: water, ethanol, and methanol. **(A)** Schematic representation of the extract preparation process from agro-industrial waste. **(B)** Methodology for the green synthesis of AgNPs assisted by LED light irradiation (450–465 nm). **(C)** Surface plasmon resonance (SPR) analysis of AgNPs by UV–Vis spectroscopy. **(D)** Morphological characterization of AgNPs by scanning electron microscopy (SEM).

The authors acknowledge the Financial support of ARES (Académie de recherche et d'enseignement supérieur). They also express their gratitude to MateriaNova and the laboratory team for their technical assistance and for providing the facilities necessary for the development of this research.

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EES - D1 - P40

Lumifilm: Luminescent downshifting films for improving photosynthetic efficiency of photo-bioreactors

Norbert J Janowicz[1], Lan Nan[1], Erwin Reisner[1], Jenny Zhang[1], Dominic S. Wright[1]
[1]University of Cambridge, UK

Photosynthesis plays a critical role in converting sunlight and carbon dioxide into essential products such as food, biomass for feed, chemical feedstock and a potential source of green energy as depicted in Figure 1 (left). Photosynthetically Active Radiation (PAR) is the region of sunlight (400-700nm) that can be absorbed by photosynthetic pigments, however despite the potential for 100% efficiency, the overall solar-to-biomass conversion remains low (>10%) with inefficient sunlight utilisation being a key bottleneck.[1] Only 28-34% of total solar energy is efficiently utilised with UV (280-400nm) and Green (500-600nm) light being largely unused by majority of photosynthetic organisms. By augmenting the RBG ratio of the incident light, the efficiency of photosynthetic process can be significantly improved by increasing light use efficiency.
Our approach (Lumifilm), Figure 1 (right), designs luminescent downshifting polymer composite films that shifts UV to red light, targeting the absorption profile of cyanobacteria. Through the optimisation of additive absorption, film opacity and surface morphology, Lumifilm-photobioreactors have shown significant improvements to up/downstream processes with increases in biomass production (x5 vs blank), oxygen evolution rate (x3 vs blank) and photocurrent generation (x130 vs blank) under 308 nm light irradiation. The optimised film demonstrated further improvements (>x2) when evaluated against an industrial prototype under the same light conditions. This development has the potential to overcome light limitation of photosynthetic technologies, bringing them one step closer to becoming the next generation sources of sustainable energy and chemical feedstock, with wider applications in enhancement of protected environment food production.

Fig.1. Summary of application areas of photobioreactors (left) and Lumifilm approach design (right).

This work was funded by the Leverhulme Trust Research Project Grant RPG-2024-309.

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EES - D1 - P41
Assessment of biochar derived from Urena lobata fibers for use in PHA-based films

Chioma Njoku[1,2,3], Michael Daramola[1], Andrej Andjelic[2], Dries Hermans[2], Mieke Buntinx[2], Wouter Marchal[2]
[1]University of Pretoria, South Africa; [2]Hasselt University, Institute for Materials Research (imo-imomec), Belgium; [3]Federal University of Technology Owerri, Nigeria

The pressing demand to preserve ecosystems has prompted researchers and manufacturers to continuously seek out eco-friendly, abundant, cost-effective, and renewable resource materials. Biomass derived from lignocellulosic materials has emerged as a superior alternative to synthetic, non-renewable fossil fuels due to its recyclability, biodegradability, and cost-effectiveness. This study aimed to assess the feasibility of using biochar from Urena lobata (Caeser weed) fibers as reinforcements at varying weight percentages (0, 0.5, 1, 3, and 5 wt%) in a poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBHHx) matrix for the development of food packaging films. Urena lobata fibers were extracted, dried, milled, sieved (to 63 µm), and pyrolyzed at 600 °C for 1 hour to produce the biochar. Mixtures of biochar and PHBHHx at different weight percentages were then extruded, cut, and compressed to produce the films, which were further characterized. The structural, tensile, and optical properties of the biochar and the produced films were investigated. Gas Chromatography-Mass Spectrometry (GC-MS) results indicated that no polycyclic aromatic hydrocarbons (PAHs) were detected in the biochar. The addition of biochar resulted in up to 18% improvement in the stiffness of the produced films; however, tensile strength and elongation at break decreased by approximately 14% and 21%, respectively, as the biochar loading increased. There was a consistent decrease (about 25 to 79%) in lightness and a rise in opacity (about 24 to 824%) with more biochar added. Biochar from Urena lobata fibers has been successfully used in making PHBHHx-based food packaging films. However, to improve the tensile strength and elongation at break of the composites, a compatibilizer such as maleic anhydride grafted polyethylene could be added during processing.

Acknowledgement: The authord acknowledge FWO, grant number V504925N, for the funding of this research project.

EES - D1 - P42
Ti4C3 and Ti4N3 MXenes for next-generation sodium ion battery anodes

Hafiz Adil Qayyum[1,2]
[1]Dept. of Physics, College of General Studies, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals, Saudi Arabia

Titanium-based materials, known for their abundance and eco-friendly nature, offer a sustainable foundation for developing next-generation energy storage materials. In this work, density functional theory (DFT) calculations are employed to systematically examine the structural, electronic, and magnetic properties of Ti-derived MXenes, Ti4C3 and Ti4N3, for their suitability as anode materials for sodium-ion batteries (SIBs). The results demonstrate that these Ti-derived MXenes possess exceptionally low Na^+ diffusion barriers, high theoretical capacity, and optimal open-circuit voltage for standard sodium-ion battery operations. Furthermore, by integrating critical performance descriptors—including average open-circuit voltage (OCV), theoretical capacity, and diffusion barrier—into a unified figure of merit (FOM), we show that these Ti-based MXenes achieve superior overall performance relative to numerous established two-dimensional anodes. Collectively, these insights highlight that Ti-based MXenes are promising candidates for advancing sustainable and efficient sodium-ion battery technologies.

EES - D1 - P43
Assessing PFAS fingerprints and precursor burden in AFFF-impacted waters and sediments

Jeonghoon Park, Kyung-Duk Zoh[1,*]
[1]Dept. of Environmental Health Sciences, School of Public Health, Seoul National University, Republic of Korea

An integrated fingerprinting framework was developed to characterize AFFF-derived PFAS contamination in surface waters and sediments at three AFFF-impacted sites in South Korea (one firefighting training facility and two air force bases). Fifty target PFAS were quantified by liquid chromatography–tandem mass spectrometry, suspects were screened by ion mobility–high-resolution mass spectrometry with collision cross section support to strengthen class-level assignment, and surface waters were subjected to the total oxidizable precursor (TOP) assay to estimate oxidizable perfluoroalkyl carboxylate (PFCA) precursors. Surface waters contained up to 7,940 ng/L ΣPFAS, with perfluorooctane sulfonate (PFOS) and perfluorohexane sulfonate (PFHxS) up to 2,133 and 1,580 ng/L, respectively, whereas sediments were dominated by long-chain perfluoroalkyl sulfonates, including PFOS up to 3,570 ng/kg□dw. Suspect screening identified 8 PFAS classes, including sulfonamide-based species typical of electrochemical fluorination (ECF) formulations and a fluorotelomer (FT) betaine observed exclusively near the Republic of Korea Air Force base. To the best of current knowledge, Class 1 bis-perfluoroalkyl sulfonimides were tentatively identified for the first time in AFFF-impacted environmental media. TOP assay results indicated large pools of unknown precursors (182–4,972 pM; 14–51 mol% of total PFAS). Ratio-based fingerprint indicators, TOP-derived precursor indices, and flow-corrected contrast metrics, interpreted together with suspect-class profiles, enabled screening-level differentiation of ECF- and FT-related signatures, prioritized PFAS hotspots at outfalls and downstream confluences across the three study areas, and quantified oxidizable precursor burdens.

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EES - D1 - P44

Toward sustainable aromatics production: Zeolite-catalyzed conversion of biomass- and CO_2-derived alcohols

Tatinaidu Kella[1], Abdullah M. Aitani[1], Hassan Alasiri[1]
[1]Interdisciplinary Research Center for Refining and Advanced Chemicals (IRC-RAC), King Fahd University of Petroleum and Minerals, Saudi Arabia

The petrochemical industry remains heavily reliant on fossil-derived aromatics, posing a significant challenge to achieving global decarbonization targets[1,2]. A promising alternative is the sustainable production of benzene, toluene, and xylenes (BTX) from renewable alcohols derived from biomass conversion and CO_2 utilization pathways coupled with low-carbon hydrogen. This review critically examines recent advances in methanol-, ethanol-, and butanol-to-aromatics chemistry, focusing on catalyst design, carbon efficiency, and long-term stability[3]. Catalyst design strategies are compared, including acidity tuning via the Si/Al ratio and framework modification, mesostructuring approaches (hierarchical porosity and nanosizing), and metal functions (e.g., Zn, Ga) that promote dehydrogenation. Across alcohol feeds, topology-acidity-diffusion relationships are discussed to explain BTX yield versus coke formation, while heavier or mixed-alcohol feeds are highlighted as additional constraints through faster condensation chemistry and transport limitations. Operando/advanced characterization (spectroscopy, microscopy, and temperature-programmed analyses) is emphasized to connect evolving active-site environments with deactivation under realistic reaction conditions. The review concludes with priorities for catalyst architectures that balance micropore shape selectivity with mesopore accessibility, and for tighter coupling of mechanistic insight to reactor/process design and TEA/LCA relevant metrics. These advances are essential to translate alcohol-to-aromatics chemistry into scalable low-carbon BTX pathways.

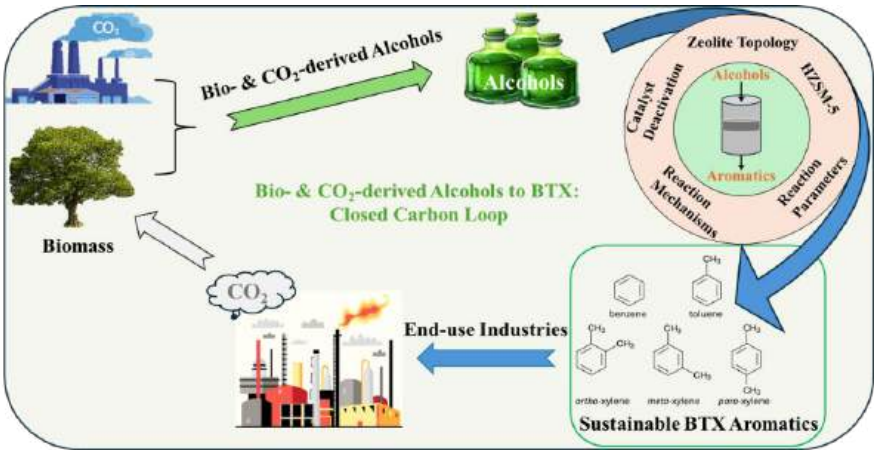

Fig. 6. Closed-carbon pathway from biomass/CO_2-derived alcohols to sustainable BTX aromatics.

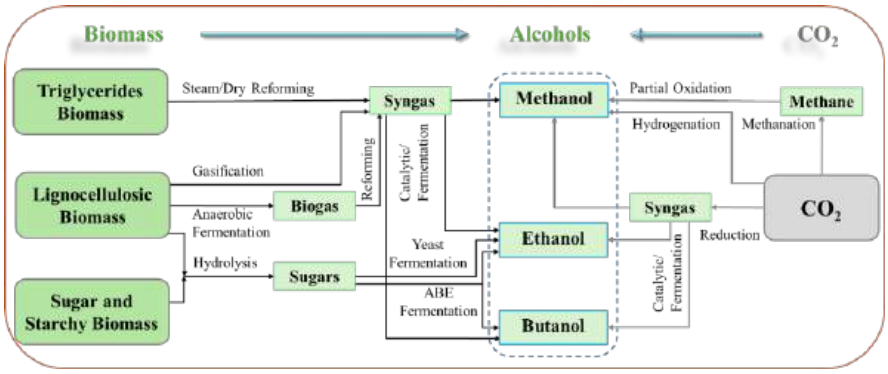

Fig. 7. Schematic representation of renewable alcohol production from biomass and CO_2 feedstocks.

Acknowledgements: This work was supported by the Interdisciplinary Research Center for Refining and Advanced Chemicals (IRC-RAC), King Fahd University of Petroleum & Minerals, Saudi Arabia.

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EES - D1 - P45

Efficient hydrogenation of CO_2 to formate by homogeneous bidentate phosphine-rhodium system

Bivas Chandra Roy[1], EA Jaseer*[1,2], Abdelrazek H. Mousa*[1,2]
[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia; [2]Dept. of Chemistry, King Fahd University of Petroleum and Minerals, Saudi Arabia

The continuous rise in atmospheric carbon dioxide (CO_2), primarily resulting from the widespread use of fossil fuels, represents one of the most pressing environmental challenges of present time. Its accumulation is directly linked to climate change, ocean acidification, and long-term ecological instability, highlighting the necessity for efficient and sustainable CO_2 valorization strategies which transform this abundant greenhouse gas into different value-added chemicals. In this context, the catalytic hydrogenation of CO_2 to formic acid (FA) has emerged as a particularly attractive approach, combining carbon utilization and reversible hydrogen storage.[1]

Formic acid is an attractive energy vector owing to its high volumetric hydrogen density, liquid nature under ambient conditions, and compatibility with existing distribution and storage infrastructure.[2] As a result, FA has emerged as a viable hydrogen carrier for fuel cells and decentralized energy applications. Despite extensive efforts in this area, the most efficient homogeneous catalysts reported to date have predominantly relied on ruthenium and iridium-based systems. In contrast, rhodium, while extensively explored in hydrogenation, hydroformylation, and C–H functionalization has remained largely underexplored for CO_2 hydrogenation. This disparity can be attributed to the comparatively lower hydricity character and greater thermodynamic stability of Rh–H bonds, which disfavor the key CO_2 insertion step relative to Ru–H and Ir–H analogues.

Herein, we report a simple yet highly effective bidentate phosphine ligand-based rhodium catalyst that displays remarkable activity and stability for the homogeneous hydrogenation of CO_2 to formate under relatively mild conditions. Importantly, to the best of our knowledge, the catalyst delivers turnover numbers that exceed all previously reported rhodium-based homogeneous systems for this transformation. These findings not only establish rhodium as a competitive platform for CO_2 hydrogenation but also provide new design principles for developing efficient hydrogenation catalysts based on alternative ligand–metal architectures.

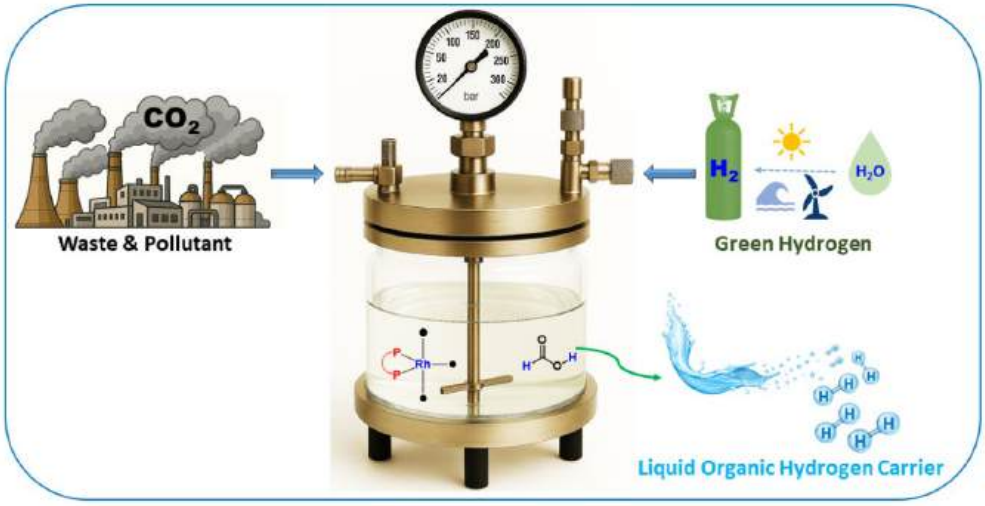

Image 1. Overview of the Significance of the Present Study

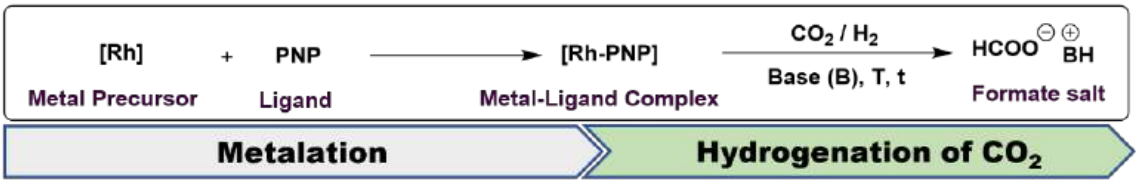

Image 2. One-top Strategy for CO_2 Hydrogenation to Formate

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EES - D1 - P46

Closed-loop chemical recycling of PET via glycolysis: Preserving structural, thermal, and molecular integrity with post-consumer waste

Zulfiqar Ahmed Rehan[1], Saqib Nasib Rana[1], Imran Hassan Syed[1]
[1]Dept. of chemistry, college of Science, Sultan Qaboos University Muscat, Oman

The rapid growth of poly(ethylene terephthalate) (PET) consumption and accumulation of post-consumer waste (PCW) necessitate efficient recycling strategies to close the loop on polymer sustainability. In this work, chemically recycled PET incorporating 0–10 wt% PCW was synthesized via melt-phase glycolysis with antimony trioxide as a catalyst and systematically characterized to assess its suitability for high-value applications. Thermal analyses revealed a slight decrease in melting temperature (247.4–246.4 °C) and consistent degradation onset (400–500 °C) across all formulations, indicating stable thermal performance. Intrinsic viscosity declined moderately from 0.743 to 0.719 dL/g, corroborated by gel permeation chromatography results showing reduced molecular weights and higher polydispersity at increasing PCW levels. Carboxyl end-group analysis confirmed trends of chain termination and partial repolymerization. Importantly, FTIR and ^{1}H NMR spectra verified backbone retention without structural degradation, while SEM, EDX, and XRD demonstrated preserved morphology, elemental purity, and semi-crystalline order. These findings confirm that chemically recycled PET containing up to 10% PCW maintains essential structural, thermal, and molecular attributes, ensuring its applicability in demanding end-uses. The results further suggest that higher PCW incorporation may be feasible with process optimization, advancing the development of sustainable closed-loop PET recycling technologies.

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EES - D1 - P47
Insight PET water bottles recycling through reactive extrusion: Conditions and processing

Amina Ouadah[1], Redouane Melouki[1]
[1]Ecole Militaire Polytechnique, Algiers, Algeria

Polyethylene terephthalate (PET) is one of the most daily used plastics in the word. Meanwhile, its upcycling reveals a processability issue. The present framework focused on the structure modification of PET issued from water bottles through reactive extrusion using a tertiary amine (triethanolamine) and epoxy diglycidyl ether bisphenol A (DGEBA) resin. The extrusion parameters have been studied in order to modify the final product properties. These investigation studies the effectiveness of this technique in converting PET waste (water bottles precisely) into new usable materials. Within the process of reactive extrusion through a twin-screw extruder, a number of parameters was experienced. The mixture composition is a trigger parameter as the percentages of introduced amine and epoxy affects significantly the cross-linked network morphology. The extrusion conditions varied for temperatures ranging from 250°C until 260°C, rotation speeds of 80 rpm and 100 rpm and extrusion times (minimum of 5 minutes and maximum of 10 minutes).
Exploring FTIR spectral analysis, reactive extrusion induces significant changes in the chemical structure of PET suggesting a chemical interaction during the process. A good thermal stability of modified PET examined through TGA was observed. XRD combined DSC confirm a semi-crystalline morphology of modified PET.
The material reveals thermal and morphological changes that are particularly interesting; at the same time a good thermal stability encouraging its use applying these parameters for second generation.

EES - D1 - P48
Ti_2C MXene–driven EMSI in Cu–ZnO catalysts for CO_2 hydrogenation to methanol

Sameera Shafi[1], Ghazali Tanimu[1,*]
[1]Center for Refining & Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia

The hydrogenation of CO_2 to methanol is a key catalytic process for closing the carbon cycle and enabling sustainable chemical production. Here, we report the development of a Cu–ZnO/Ti_2C@Ti_2O_5 catalyst that exploits a strong electronic metal–support interaction (EMSI) enabled by a Ti_2C MXene-derived support with abundant unsaturated Ti sites. Spectroscopic analyses (XPS), temperature-programmed reduction, and density functional theory calculations collectively demonstrate pronounced electron donation from surface Ti species to Cu nanoparticles, generating an electron-rich Cu interface that enhances CO_2 activation. Adsorption studies using H_2-TPD and CO_2-TPD reveal that exposed Ti sites substantially improve the activation of both reactants, leading to enhanced catalytic efficiency. As a result, the catalyst delivers a methanol formation rate of 235 mg (g_cat h)$^{-1}$ with 72.1% selectivity at 240 °C and 3 MPa, while maintaining excellent structural integrity and stable performance during 60 h of continuous operation**.** Mechanistic insights indicate that strong CO* binding at the Ti–Cu interfacial sites promotes a reaction pathway dominated by the RWGS-derived CO hydrogenation route**,** thereby favoring methanol synthesis. This work underscores the potential of MXene-based supports for tailoring EMSI and interfacial adsorption properties, offering a general design principle for high-performance CO_2 hydrogenation catalysts.

Acknowledgement: Center for Refining & Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran

EES - D1 - P50
Valorization of textile waste through enzymatic processes

Bruna Fernandes[1], Bruno Godinho[1], Nuno Gama[1], Artur Ferreira[1]
[1]CICECO – Aveiro Institute of Materials and University of Aveiro, Portugal

The increase in production and disposal of post-consumer textile waste (PCTW), driven by fast fashion, represents an urgent environmental challenge, with millions of tonnes of complex fiber blends such as cotton, polyethylene terephthalate (PET), polyacrylonitrile (PAN), and thermoplastic polyurethane (TPU) annually destined for landfilling.[1] Conventional recycling methods (mechanical, chemical, and thermal) are often non-selective, energy-intensive, and environmentally damaging, leading to downcycling or the generation of hazardous effluents.[1] This research proposes the development of a sustainable recycling methodology based on selective enzymatic depolymerization for the valorization of complex textile mixtures.[2] The project aims to address a critical knowledge gap by testing specific enzymes (cellulases, cutinases, and nitrilases) on mixed waste streams, including challenging polymers like PAN and polyvinyl chloride (PVC).[3] Through the application of tailored pretreatment strategies to enhance accessibility and subsequent sequential enzymatic action, this methodology seeks the efficient separation and recovery of high-value monomers, as well as the surface modification of recalcitrant polymers.[3] The results are expected to establish a proof-of-concept for a closed-loop bioconversion process, promoting circularity and reducing the environmental footprint of the textile value chain.

Funding: This work was conducted within the scope of the PRR Mobilizing Agenda “GreenAuto – Green Innovation for the Automotive Industry”, funded by the PRR – Recovery and Resilience Plan and co-funded by NextGenerationEU through the “Agendas for Business Innovation” scheme.

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EES - D1 - P64

Upgrading date palm-derived organosolv lignin oil into cycloalkanes for sustainable aviation fuel (SAF) via Ni-based bifunctional catalysis

Nazia Siddiqui[1], Abdulkadir Tanimu[1], Niladri Maity[1], Konstantinos S. Triantafyllidis[1,2,3*]

[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia; [2]Chemistry Dept., KFUPM, Saudi Arabia; [3]Saudi Aramco Chair in Catalysis and Petrochemicals, KFUPM, Saudi Arabia

The sustainable utilization of lignocellulosic residues provides a strategic route to lowering dependence on fossil-based fuels, including aviation fuels. Waste date palm, widely available in Middle East regions-particularly Saudi Arabia offers an abundant source of biomass with strong potential for conversion into aromatic or cycloalkane hydrocarbons, especially via utilization of its lignin structural component. In this work, an integrated process is presented that comprises of the selective extraction of lignin from date palm biomass via tailored organosolv fractionation followed by depolymerization via hydrogenolysis or solvothermal liquefaction to obtain lignin oil enriched in syringol and guaiacol-type alkoxy-phenolic monomers and oligomers. Catalytic upgrading of this lignin oil was systematically investigated via hydrodeoxygenation (HDO) with bifunctional, non-sulfided, nickel (Ni)-based catalysts supported on zeolites. The HDO reaction of representative lignin-derived model compounds, including alkoxy/alkyl-phenols and alkoxy-aromatics was studied to identify the reaction mechanism and how it is affected by the phenolic ring substitution. A generic HDO mechanism was identified, comprising of the following steps: phenolic compound → cyclohexanone → cyclohexanol → cyclohexene → cyclohexane, utilizing the hydrogenation function of Ni and the alcohol dehydration acidic function of the zeolite support. In general, small phenolics, like phenol and anisole were easily hydrodeoxygenated at low temperatures, ca. 220^{o}C, but by increasing the complexity of the aromatic ring with methoxy, alkyl and aldehyde side groups, higher temperatures were needed to achieve pronounced deoxygenation. To this end, the real lignin oil HDO, due to the presence of oligomers as identified by 2D HSQC NMR, required relatively high temperature (300-400^{o}C) to obtain deoxygenation as high as 90%, towards respective C6-C9 alkyl-aromatic and cycloalkanes.

The support of Postdoctoral Research Fellowship Program and Interdisciplinary Research Center for Refining and Advanced Chemicals, KFUPM is gratefully acknowledged. K.S.T. also acknowledges the Deanship of Research, KFUPM for support received under Grant no. CUP24201.

EES - D1- P65

$Ni/LaMnO_3$ perovskite catalysts promoted by alkali and alkaline earth metals for green hydrogen generation via NH3 decomposition

Ahsan Ali[1], M. Nasiruzzaman Shaikh[1]

[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia

Chemical hydrogen carriers such as ammonia (NH_3) have garnered increasing attention. NH_3 is a carbon-free compound with a high hydrogen content (17.6 wt.%), can be liquefied at -33.3 °C under ambient pressure, and benefits from an established global infrastructure for production and transport. Importantly, it can be catalytically decomposed into nitrogen and hydrogen, enabling CO_2-free, on-demand hydrogen production.

In this study, $LaMnO_3$ was synthesized via a sol-gel method and employed as a perovskite support for Ni-based catalysts. A series of alkali and alkaline earth metal promoters (K, Cs, Sr, Ca, In) were incorporated to investigate their impact on catalytic activity and physicochemical properties. Structural and surface analyses (XRD, SEM-EDS, TEM, BET, XRF, H_2-TPR, and CO_2-TPD) confirmed the successful integration of promoter elements without compromising the perovskite structure. NH_3 decomposition was studied in a fixed-bed tubular reactor. The experimental setup consisted of a stainless-steel (316) tube reactor (12.7 mm i.d., 280 mm length) integrated with a furnace, heater, flow controllers, gas supply lines (10% NH_3/He, H_2, and He), and an online GC.

Catalytic testing revealed that unpromoted Ni/LaMnO3 achieved 90% NH_3 conversion only at 640 °C, highlighting the need for further enhancement. Among all samples, the 3%K-$Ni/LaMnO_3$ catalyst demonstrated superior performance, achieving 90% conversion at 530°C and complete decomposition at 630 °C. K promotion significantly increased the surface area and porosity, enhanced the reducibility of Ni species, and improved surface basicity. Optimization of K loading revealed that 3 wt.% was optimal, with higher concentrations leading to a slight decline in performance. Long-term stability evaluation at 600 °C for 24 h confirmed sustained catalytic activity and structural integrity. The observed catalytic activity followed the trend: 3%K-$Ni/LaMnO_3$ > 3%Cs-$Ni/LaMnO_3$ > 3%Sr-$Ni/LaMnO_3$ > 3%In-$Ni/LaMnO_3$ > 3%Ca-$Ni/LaMnO_3$ > $Ni/LaMnO_3$, and these results elucidate the critical role of K in enhancing the performance of $Ni/LaMnO_3$ catalysts.

EES - D1 - P66

Accelerated LiF/HCl etching for rapid MXene synthesis beyond Ti_3AlC_2

Ata-ur-Rehman[1], Muhammad Mansha[1], Safyan Akram Khan[1], Muhammad Nawaz Tahir[1], Shahid Ali[1,*]
[1]*Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum and Minerals, Saudi Arabia*

The synthesis of MXenes remains challenging, particularly for MAX phases beyond titanium-based systems. Among existing methods, LiF/HCl etching has emerged as the most versatile approach, initially optimized for Ti_3AlC_2 and later extended to mixed-metal (e.g., $Mo_2Ti_2AlC_3$) and non-titanium (e.g., V_2AlC) MAX phases, enabling the production of large-area, high-quality MXene sheets. Despite these advances, conventional LiF/HCl etching suffers from two major limitations: prolonged reaction times (≥ 24 h) and degradation of the resulting MXenes, which compromise structural integrity and practical applicability. Herein, we report a markedly accelerated MXene synthesis strategy, achieving almost complete etching within **2 h at 140 °C**, representing the first demonstration of such rapid LiF/HCl-based processing. This shortened etching time significantly suppresses oxidation while maintaining high product yields. Under optimized conditions, etching efficiencies of **74%, 86%, and 92%** were achieved for **Ti_3C_2, V_2C, and $Mo_2Ti_2C_3$**, respectively. The resulting products were readily delaminated into few-layer MXene sheets after only a few minutes of ultrasonication, underscoring the efficiency of the method.
Comprehensive structural and chemical characterization by XRD, SEM, TEM, and XPS confirmed successful MAX phase conversion, layered MXene morphologies, and preservation of metal–carbon bonding. Furthermore, dynamic light scattering and zeta potential analyses revealed excellent colloidal behavior, with the MXene dispersions exhibiting **months-long stability** without noticeable degradation. The combination of dramatically reduced processing time, suppressed oxidation, and robust colloidal stability represents a significant step toward scalable MXene production and broadens their potential for long-term applications in energy storage, catalysis, and related advanced technologies.

Acknowledgement: The authors would like to acknowledge the financial support received from “King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia” to conduct this research work under the IRC-HTCM project # INHT2421.

EES - D2 - P01

From materials development to system integration: Photoanode surface activation and validation of a continuous-flow PEC device for efficient solar hydrogen production

Anthony Sanderse[1*], Amir Shokir[1], Jorgen Sweelssen[1], Jonathan van den Ham[1], Nicole Meulendijks[1], Pascal Buskens[1,2]

[1]The Netherlands Organisation for Applied Scientific Research (TNO), The Netherlands; [2]Hasselt University, Belgium

Hydrogen is a key enabler for decarbonizing society, serving as both a renewable energy carrier and a feedstock for chemical processes beyond electrification. To compete with fossil-based hydrogen, green hydrogen must be produced at large-scale and lower costs. Photoelectrochemical (PEC) water splitting has the potential to lower prices substantially, resulting from cost-effective, abundant electrode materials and integrated device design. While materials like $BiVO_4$, Fe_2O_3, and Si are effective photoanodes, their bare surfaces exhibit limited activity in the oxygen evolution reaction (OER) and are prone to rapid deactivation from photocorrosion.[1]

Here, we functionalize the surfaces of several photoanodes with bimetallic NiFeOOH electrocatalysts, significantly improving OER kinetics and mitigating photocorrosion. These photoelectrode degradation effects typically occurs within a few hours of operation, but batch PEC reactors limit long-term testing abilities due to poor mass transport and bubble accumulation. We present a modular continuous-flow PEC (flowPEC) reactor, inspired by electrolyzer technology, that enables long-term performance validation of PEC materials and advances the technological readiness of PEC systems.

Loading the photoanodes with NiFeOOH electrocatalysts increases the photocurrent under alkaline conditions by 50-500% compared to the pristine photoanodes and reduces the overpotential by 300 mV or more. In the flowPEC reactor, NiFeOOH-loaded photoanodes exhibit stable long-term performance while bare photoanodes degrade rapidly. Without a guided flowfield, apparent deactivation of the PEC performance was related to bubble adhesion, rather than photoelectrode failure. Efficient gas removal was achieved by tailoring the flowfield channel size, allowing stable performance over 5 hours.

The continuous flow-PEC device provides a suitable platform to analyse intrinsic catalytic performance and long-term stability of photoanodes, supporting the development of scalable, sustainable hydrogen production.

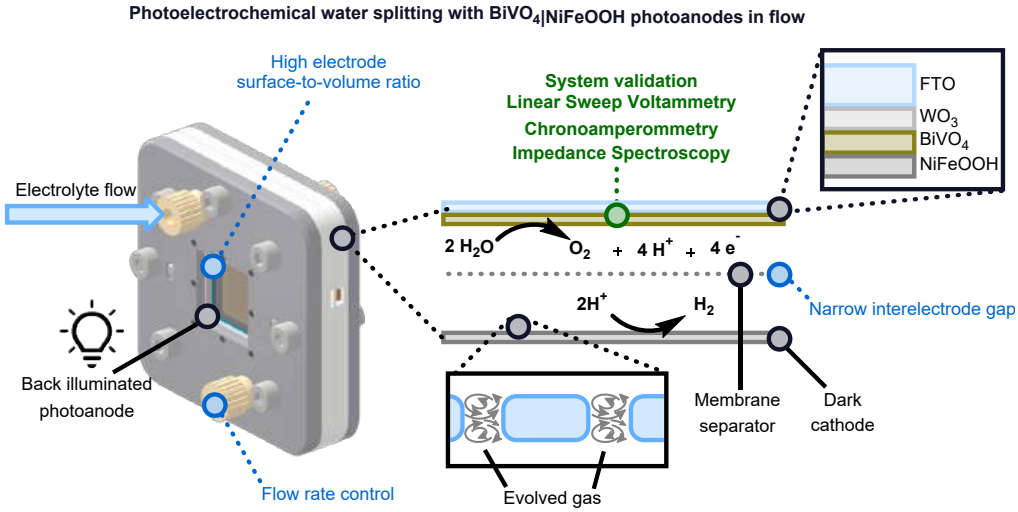

Fig. 1. Design of the flowPEC reactor and application thereof in the sunlight-driven water splitting reaction using $BiVO_4$-based photoanodes.

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EES - D2 - P01

Comparative study on the inhibitory effectiveness of plant extracts against corrosion of a metal alloy

Abdeldjalil Aimen Kaidi[1], Sana Tazibet[1], Amina Ouadah[1], Sofia Benamirouche[1]
[1]Electrochemistry and corrosion laboratory, Polytechnic military school CHAHID ABDERRAHMANE TALEB, Algeria

The corrosion of metallic materials represents a major industrial and economic challenge, as well as a source of significant environmental concerns. Conventional corrosion inhibitors, while effective, often consist of heavy metals (chromates) or toxic and non-biodegradable synthetic molecules, the use of which is increasingly regulated. Faced with this ecological imperative, research is turning towards the development of sustainable and environmentally friendly alternatives, based on the principles of green chemistry. This study aims to evaluate the effectiveness of new biosourced corrosion inhibitors, derived from natural plant extracts (Pistacia lentiscus and Olea europaea) using an optimized extraction method (ultrasound-assisted extraction), for the protection of carbon steel (XC38) in an acidic medium (0,5M HCl). The methodological approach combines a quantitative analysis (gravimetric) with advanced electrochemical techniques (electrochemical impedance spectroscopy - EIS, potentiodynamic polarization) and surface analyses (SEM, FTIR spectroscopy, optical microscope) to characterize the inhibition mechanism. Preliminary results demonstrate remarkable inhibition efficiency (percentages that can reach up to 90%) at an optimal concentration of 300 ppm (mass of the extract in acidic solution). Electrochemical analysis suggests that these compounds primarily act as mixed type inhibitors, forming a protective adsorbed film on the metal surface. These findings confirm the potential of green inhibitors as viable and high-performing substitutes for toxic synthetic inhibitors. The results open promising perspectives for the industrial application of these ecological solutions, thereby contributing to a more sustainable metallurgical industry.

Keywords: Corrosion Inhibition, Plant Extracts, Carbon Steel, Acidic Medium, Inhibitory Effectiveness.

EES - D2 - P03
Electrified adsorptive separation of fermentative iso-butyric acid

Azam Aydani[1], Hafez Maghsoudi[1], Mohsen Gholami[1], Keikhosro Karimi[1], Joeri Denayer[1]
[1]Vrije Universiteit Brussel, Belgium

Iso-butyric acid (IBA) is a high value C4 carboxylic acid with a rapidly growing market[1]. The sustainability and market demand of bio-based products have shifted attention to fermentative synthesis of IBA using renewable biomass[2]. Inefficient downstream processes prevents the industrial use of bio-based IBA due to the potential of recovering dilute acids in complex fermentation broths consuming up to 60% of overall production costs[3]. Traditional techniques of separation have many drawbacks such as energy-intensive processes, solvent toxicity, fouling, and low selectivity[4]. Therefore, adsorption has become a potential alternative due to its high selectivity, mild operation conditions and compatibility with aqueous systems.
Zeolites with high Si/Al ratio like ZSM-5 possess a high affinity to C4 carboxylic acids due to their hydrophobicity. However, the regeneration based on traditional thermal swing adsorption is still energy consumptive[5]. Electrified swing adsorption (ESA), involving direct Joule heating, provides rapid heating, high precision temperature control and better energy efficiency. Despite the extensive application of ESA in gas-phase separations, its application in liquid-phase systems remains limited.
This study investigates employing a hydrophobic ZSM-5 zeolite hybrid monolith for IBA separation and recovery from aqueous solutions using dynamic breakthrough experiments, as well as the efficacy of ESA regeneration process. Dynamic breakthrough experiments demonstrate efficient IBA adsorption, on the hybrid monolith. Moreover, ESA regeneration effectively desorbed the adsorbed IBA. The results indicates this method can selectively recover IBA in aqueous media, which could serve to provide scalable and energy-efficient downstream technology in biorefinery.

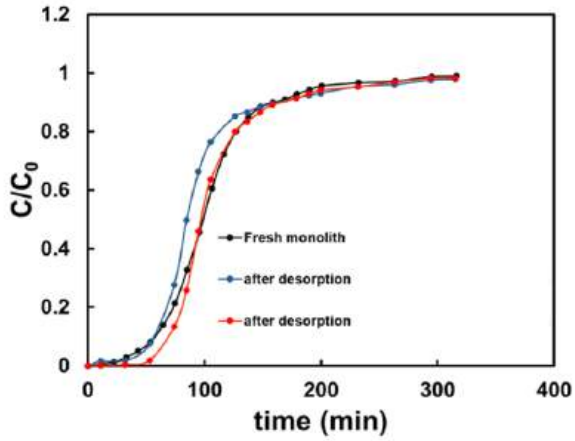

Fig. 1. Breakthrough experiment results before and after regeneration through ESA process.

Acknowledgements: This work was supported by the Research Foundation - Flanders (FWO) through the Thematic Research Project *Effective*.

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EES - D2 - P04
Optimization of TPU recycling processes used in the ceramic industry

Sofia Caldas[1], Inês Almeida[1], Patrícia Mata[2], Shantanu Wahane[2], Luís Tarelho[2], Flávio Azedo[3], Jorge Marinheiro[3], Ana Barros Timmons[1], Nuno Gama[1]
[1]Dept. of Chemistry, University of Aveiro, Portugal; [2]Dept. of Environment and Planning, University of Aveiro, Portugal; [3]Porcelanas da Costa Verde S.A., Portugal

Polyurethane (PU) consumption continues to grow, intensifying concern about the management of the resulting waste [1]. In response to this challenge, there has been a growing trend toward developing recycling technologies aimed at recovering reusable raw materials, thereby promoting the circular economy. Within this context, acidolysis has emerged as a promising depolymerization strategy, widely investigated for the recycling of PU foams [2]. However, despite its relevance, the application of acidolysis to thermoplastic polyurethane (TPU) remains largely unexplored. This study addresses this gap by investigating the chemical recycling of TPU residues generated from ceramic production, using succinic acid as the cleavage agent. The depolymerization mechanisms were examined through Fourier Transform Infrared (FTIR) spectroscopy, ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectroscopy and Gel Permeation Chromatography (GPC), and the influence of temperature, reaction time and PU/acid molar ratio on the acid value (AV), hydroxyl value (IOH), and molar mass ($\bar{M}_w$) of the recycled polyol (RP) was evaluated. Finally, the potential of the RP is assessed through its incorporation into new TPU formulations, revealing its suitability for partial substitution of commercial polyol without compromising key thermal and mechanical properties. Overall, this study expands the application range of acidolysis to a new class of PU waste and outlines a viable circular pathway for TPU residues from the ceramics industry.

Funding: This research was funded by FEDER – Fundo Europeu de Desenvolvimento Regional funds through of Programa Inovação e Transição Digital in the scope of the project “CiPoCer”, CENTRO2030-FEDER-01169500, and was developed within the scope of the project CICECO – Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020) & LA/P/0006/2020 (DOI10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

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EES - D2 - P05
Functionalized cyclodextrin materials for advanced PFAS removal

Pavlína Konopáčová[1,2], Christopher Hobbs[2], Martin Stuchlík[2], Michal Řezanka[2]
[1]Faculty of Science, Humanities and Education, Technical University of Liberec, Czech Republic; [2]Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, Czech Republic

Poly- and perfluoroalkyl substances (PFAS) are persistent synthetic chemicals widely used in industrial and consumer applications due to their unique stability and surface-active properties. Their carbon–fluorine bond makes them highly resistant to degradation, leading to widespread environmental contamination and accumulation in aquatic systems. PFAS exposure poses serious health risks, including carcinogenic and reproductive problems,[1] while conventional water treatment technologies fail to remove them effectively.[2]
Sorption-based strategies have emerged as promising solutions for PFAS remediation. Cyclodextrins, cyclic oligosaccharides with a hydrophobic inner cavity and hydrophilic outer surface, can selectively form host–guest complexes with hydrophobic molecules, providing a molecular-level mechanism for capturing contaminants.[3]
The versatility of cyclodextrin–based materials can be further enhanced by introducing positively charged groups, which promote electrostatic interactions with anionic PFAS.[4] In this work, we develop insoluble materials functionalized with cyclodextrins, using a range of cross-linking strategies. These approaches allow precise tuning of polymer structure, porosity, and surface chemistry to maximize PFAS binding. The resulting materials combine selective molecular recognition with environmental compatibility, offering a sustainable and practical solution for water purification. Cyclodextrin–based materials represent a promising class of sorbents capable of improving the removal of PFAS from contaminated water and supporting safer drinking water and wastewater treatment systems. Preliminary results on the synthesis and characterization of these materials, as well as their PFAS-binding potential, will be presented at the conference.

This work was supported by the Student Grant Competition of the Technical University of Liberec under the project No. SGS-2024-4440.

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EES - D2 - P06

Pollen-templated cu and Ni@Cu (photo)catalysts for sustainable degradation of pharmaceutical pollutants

Gonzalo García [1,2], Jordi Rigual-Miret [1,2], Elvira Gómez [1,2], Albert Serrà [1,2]*

[1]Dept. de Ciència de Materials i Química Física, Universitat de Barcelona, Spain; [2]Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Spain

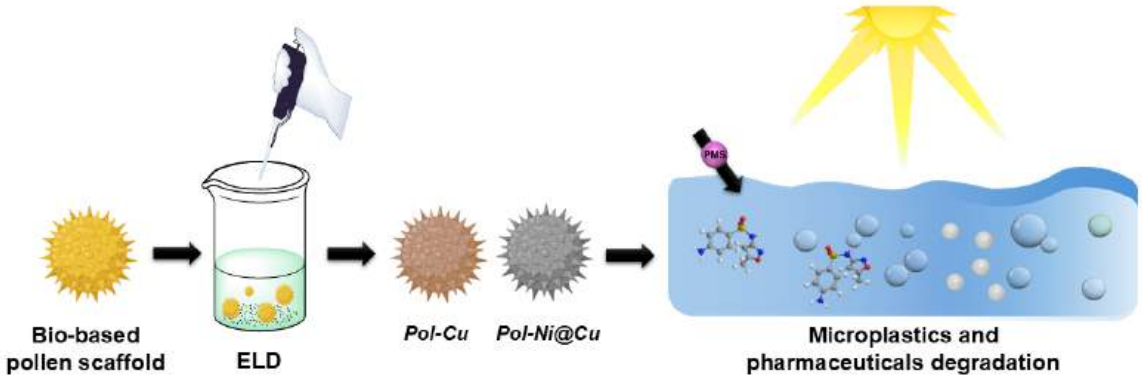
Bio-derived scaffolds offer a sustainable platform for the development of advanced (photo)catalysts, combining low environmental impact with hierarchical architectures, high surface area, and good structural stability. Among these, pollen grains constitute an abundant and renewable natural template that can be directly exploited for catalyst synthesis.

In this work, pollen grains of *Chrysanthemum leucanthemum* were employed as templates for the preparation of metal-based catalysts via electroless deposition (ELD). Two materials were synthesized: a copper-coated pollen catalyst (Pol-Cu) and a bimetallic nickel–copper catalyst (Pol-Ni@Cu), obtained by nickel deposition onto a pre-formed copper layer. The resulting materials preserve the hierarchical morphology of the pollen scaffold while incorporating catalytically active metallic phases.

The (photo)catalytic performance of the catalysts was evaluated for the degradation and mineralization of pharmaceutical pollutants in water, using sulfamethoxazole (SMX) as a model compound. Catalytic activity was enhanced by peroxymonosulfate (PMS) addition, enabling the generation of reactive oxygen species. A systematic study examined the influence of pH, catalyst loading, initial SMX concentration, and illumination conditions (visible light versus dark).

Both catalysts showed effective SMX degradation and mineralization, with Pol-Ni@Cu consistently outperforming Pol-Cu. Under visible light irradiation, Pol-Ni@Cu exhibited enhanced activity, indicating photo-assisted PMS activation. After 120 min, maximum mineralization efficiencies of 83.0% and 91.3% were achieved for Pol-Cu and Pol-Ni@Cu, respectively. Variations in operational conditions produced consistent trends in degradation and mineralization, highlighting the synergistic effects of catalyst composition and light irradiation.

To assess environmental relevance, the catalysts were tested in a multicomponent system containing sulfamethoxazole, tetracycline, ibuprofen, and levofloxacin, maintaining high mineralization efficiencies. Ongoing studies extend the application of Pol-Ni@Cu catalysts to microplastic degradation, reinforcing their potential for sustainable water treatment.



Acknowledgements: Grant CNS2024-154690 funded by MICIU/AEI/10.13039/501100011033 and, as appropriate, by “ESF Investing in your future”, by “ESF+” or by “European Union NextGenerationEU/PRTR”. The authors also would like to express their gratitude to the Departament de Recerca i Universitats, particularly the Departament d'Acció Climàtica, Alimentació i Agenda Rural, as well as the Fons Climàtic de la Generalitat de Catalunya (project 2023 CLIMA 00009 AGAUR) for their support. Authors thank the CCiT-UB for the use of their equipment.

EES - D2 - P07
Impactive: European mechanochemists develop greener pharmaceuticals

Evelina Colacino[1,*], Juan José Sáenz de la Torre[2], Leyre Flamarique[2], Fernando Gomollon-Bel[2]
[1]ICGM, Univ Montpellier, CNRS, ENSCM, France; [2]Agata Communications, Santander, Spain

Mechanochemistry uses mechanical force to drive chemical reactions. In the past few years, this field has experienced a resurgence in Europe, in part thanks to the support of EU-funding bodies to different collaborative initiatives and networks,[1] but also thanks to the additional awareness about the environmental impact of chemistry.[2] In 2022, the international project IMPACTIVE kicked off with a clear goal: making mechanochemistry a manufacturing reality in pharma. The most optimistic predictions expect an 85% reduction in the ecotoxicity of pharmaceutical production, including a significant reduction of energy consumption and carbon emissions, as well as production costs. With almost €8 million in funding from Horizon Europe, IMPACTIVE gathers 17 partners, including key industries like Merck and Novartis, to ensure efficient technology transfer and early-adoption of the green chemistry and mechanochemistry solutions developed. The poster will present the overall goals of the project, which include the implementation of scalable mechanochemical methods (ball milling, extrusion, resonant acoustic mixing) to make the synthesis of antidiabetic, antihypertensive and anticancer drugs as well as formulation greener, in line with the 12 principles of green chemistry[3,4] and the United Nations Sustainable Development Goals.[5] Additionally, the move to mechanochemistry will contribute to solving the supply chain shortage problems, improving the production of drugs during emergencies. The IMPACTIVE project will contribute to the chemistry community in Europe with innovative green synthetic methodologies and catalyse commercialisation.

Acknowledgements: The authors acknowledge IMPACTIVE (Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients), the research project funded from the European Union's Horizon Europe research and innovation programme (European Health and Digital Executive Agency) under grant agreement No. 101057286. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or (European Health and Digital Executive Agency). Neither the European Union nor the granting authority can be held responsible for them.

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EES - D2 - P08

Enhancing hydrogen production and CO_2 photoreduction efficiency using 1D TiO_2 based materials

Alexandra C. Iacoban[1,2], Hussein Badr[3], Andrei Kuncser[1], Florentina Neatu[1], Stefan Neatu[1], Michel W. Barsoum[3], Mihaela Florea[1,2]

[1]National Institute of Materials Physics, Romania; [2]Interdisciplinary School of Doctoral Studies, University of Bucharest, Romania; [3]Drexel University, USA

The global energy crisis caused by fossil fuel depletion and environmental pollution underlies the urgent need to find renewable alternative energy sources. Hydrogen obtained through the photocatalytic water splitting process represents a promising solution[1], while photocatalytic CO_2 photoreduction represents an alternative for greenhouse gas emissions while generating value-added solar fuels. The limited number of semiconductor photocatalysts that combine low cost, visible-light response, long-term stability, and high efficiency remains a major challenge. An effective strategy to overcome these challenges is the design of innovative 1D materials. Their elongated morphology facilitates directional charge transport, reducing recombination losses and improving photocatalytic efficiency.

In this study, one-dimensional lepidocrocite (1DL) TiO_2 was prepared through a bottom-up, inexpensive, and scalable process, using titanium diboride (TiB_2) as precursor and tetramethylammonium hydroxide (TMAOH) at 80˚C/ 5 days, followed by further washing with EtOH or LiCl solution[2]. Small amounts of gold were further deposited using the urea-assisted deposition-precipitation method to act as a co-catalyst[3]. Photocatalytic hydrogen production and CO_2 photoreduction experiments were performed under UV-Vis irradiation.

ICP-MS analysis reveal that both 1DL materials contain very low Au amounts, ≈0.03%, attributed to their ion-exchange characteristics and limited capacity to strongly bind Au species during the deposition, while the Au/TiO_2 P25 sample shows almost ten times higher Au concentration. Despite this, the Au-modified 1DL photocatalysts exhibit enhanced hydrogen production rates due, most probably, to the presence of Au^0, and $Au^{\delta+}$ species on the surface identified by XPS. While Au/TiO_2 P25 presents mostly metallic Au^0, both 1DL samples exhibit a significantly higher fraction of $Au^{\delta+}$, indicative of strong metal–support interactions, that facilitate efficient charge separation, interfacial electron transfer, suppressing recombination, enhancing photocatalytic performance with high stability over time (Figure 1) compared to their supports[4]. Additionally, 1DL TiO_2 present a higher efficiency for CO_2 photoreduction reaction.

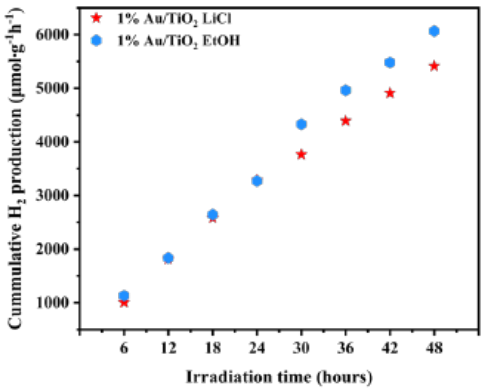

Fig. 1. Cumulative hydrogen production over time

This work was supported by financial support from the Romanian Ministry of Research, Innovation and Digitization through the Core Program 2023–2026 (contract PC3-PN23080303) and PTE 46/2025.

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EES - D2 - P09
Novel $BaTiO_3$- and $BaFeO_3$-based electrode materials for SOFCs

Valerie Theuns[1], Donovan Ledru[2], Marie-Hélène Chambrier[2], Aurélie Rolle[1], Anne-Sophie Mamede[1], Héloïse Tissot[1], Elise Berrier[1]
[1]Univ. Lille, CNRS, UCCS – Unité de Catalyse et Chimie du Solide, France; [2]Univ. Artois, CNRS, Centrale Lille, Univ. Lille, France

A key challenge in solid oxide fuel cell (SOFC) electrode development is reducing reliance on critical raw materials (CRMs), like Co, La and Sr[1], while maintaining electrochemical performance. However, non-critical alternatives like $BaTiO_3$ (BTO) show lower activity. Due to the flexibility of the ABO_3 perovskite structure, this work explores A- and B-site cation substitution to enhance redox activity and ionic conductivity, while examining the resulting structural and surface properties[2].
$BaTiO_3$- and $BaFe0_3$-based materials were synthesized via citrate autocombustion. A-site substitutions (Na^{1+}, Ca^{2+}, La^{3+}), B-site substitutions (Ni^{2+}, Fe^{3+}, Cu^{2+}) and A-site deficiency were investigated.
Characterization included SSA, TGA-DSC, TPR-TPO, XRD, Raman spectroscopy, XPS, NAP-XPS and EIS. *In-situ* Raman measurements were performed using multiple excitation wavelengths. Quasi *in-situ* XPS was conducted after thermal treatment under reactive gas flow, and UHV transfer. NAP-XPS measurements were carried out at 1 mbar. EIS measurements were performed with 10mV perturbation at 650°C and 800°C.
XRD, Raman, and XPS analyses revealed ex-solved crystalline phases in selected compositions. $Ba_{0.85}Ca_{0.15}Ti_{0.80}Fe_{0.20}O_3$ (B85CTF-20) showed reducibility under H_2, confirmed by TPR and *in-situ* Raman spectroscopy during H_2/O_2 cycling. H_2-TPR induced spectral modifications beyond thermal effects, Fig. 1, including a shift to lower frequencies, decreased intensity at 505 cm^{-1}, and increased intensity at 730 cm^{-1}. O_2-TPO restored the initial Raman spectrum, indicating reversible redox behaviour. Quasi *in-situ* XPS, Fig. 1, revealed metallic Fe formation after reduction at 800 °C, which disappeared upon reoxidation, linking reducibility to Fe cations. Similar characterizations were performed on La-doped samples. EIS results of $Ba_{0,85}La_{0,15}Ti_{0,80}Fe_{0,20}O_3$ (BLTF-20) showed promising polarization resistance of 4.66 Ω*cm² at 800°C for B85LTF-20.

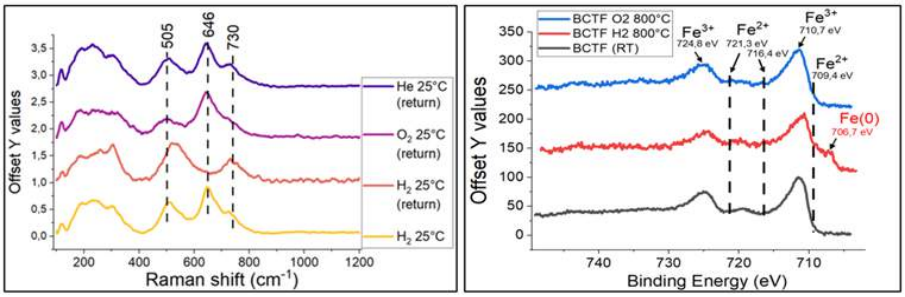

Fig.1. Left: in-situ Raman spectra at λ = 633 nm of B85CTF-20. Right: quasi in-situ XPS spectra of the Fe 2p state of B85CTF-20

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EES - D2 - P10
Mechanochemical amidation for sustainable agrochemical synthesis

Andrea Casagrande[1,2], Christos M. Chatzigiannis[1], Allan Niidu[2], Evelina Colacino[1]
[1]Institut Charles Gerhardt (ICGM), Université de Montpellier, France; [2]Virumaa Kolledž, Tallinna Tehnikaülikool, Estonia

Mechanochemical amidation represents a solvent-free synthetic strategy for the preparation of amide-containing agrochemicals through coupling of aromatic carboxylic acids and anilines. By using new generation solid-state activating agents1, marketed fungicides and phytopharmaceutical were prepared by both ball-milling and Resonant Acoustic Mixing (RAM), with higher productivity and lower environmental impact compared to synthetic strategies in solution. The mechanochemical set up circumvents the need for bulk organic solvents and hazardous reagents typical of conventional solution-based protocols, instead leveraging controlled mechanical energy input to drive the transformation. The fine tuning of the mechanochemical processing parameters allowed to maximize conversion and yields, while minimizing waste. Quantitative sustainability assessment of the mechanochemical processes was conducted by green chemistry metrics (e.g., DOZN 3.02 and CHEM213 tools), demonstrating a better eco-footprint of ball-milling and RAM-activated processes, positioning mechanochemical amidation as a viable and scalable approach aligned with sustainable chemistry principles for the manufacture of agrochemical active ingredients.

Acknowledgements: A.C. is grateful to Campus France and Tallinn Technological University (TalTech) for the Ph.D. fellowship (co-tutelle de thèse France-Estonie). E.C. and A.N. are grateful to Campus France and French-Estonian Cooperation Programme Hubert Curien France-Estonia (PHC PARROT 2021-2023). A.N. is grateful to the French Embassy in Estonia for the mobility grant (2024).

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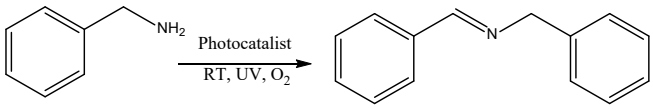
EES - D2 - P11

Photocatalytic homocoupling of benzylamines under ambient and green conditions using naturally derived photocatalyst and solvent

Antonio Monopoli[1], Tommaso Castiglia[1], Angelo Nacci[1]
[1]Università degli Studi di Bari Aldo Moro, Chemistry Dept., Italy

The homocoupling of benzylamines to form symmetric imines is a valuable transformation in organic synthesis, yielding important intermediates for pharmaceuticals, dyes, and fine chemicals. Conventional methods for this reaction often suffer from significant drawbacks, including the use of harsh oxidants, elevated temperatures, stoichiometric metal reagents, and the formation of undesired by-products such as aldehydes or nitriles, which limit substrate scope, selectivity, and sustainability. In contrast, photocatalysis has emerged as an effective strategy to address these challenges, enabling oxidative coupling under milder, light-driven conditions while often employing molecular oxygen as a benign oxidant[1-3].

Herein, we report a viable photocatalytic homocoupling of benzylamines under green and mild conditions using a naturally derived photocatalyst and green solvent. This approach minimises waste, avoids hazardous chemicals, and provides a selective, energy-efficient, and environmentally friendly route to symmetric imines, aligning with the principles of green chemistry and expanding the scope of practical synthetic applications.



We strongly acknowledge “Fondo per la Qualità e l’Internazionalizzazione della Ricerca” (issued by D.R. No. 2924 on 29/07/2024), financed by the University of Bari Aldo Moro.

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EES - D2 - P12

Metallic Cu–Ni nanoinclusions for simultaneous electrical enhancement and thermal suppression in $Bi_2Te_{2.7}Se_{0.3}$ thermoelectric thin films

Yakubu Sani Wudil[1,2]
[1]Laser Research Group, Physics Department, King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia; [2]Interdisciplinary Research Center for Construction and Building Materials, King Fahd University of Petroleum and Minerals, Saudi Arabia

The thermoelectric properties of $Bi_2Te_{2.7}Se_{0.3}$ thin films were systematically improved by introducing Cu–Ni metallic nanoinclusions during pulsed laser deposition. Reference films consisting of pristine $Bi_2Te_{2.7}Se_{0.3}$ and films containing only Cu or Ni were prepared to clarify the individual and combined effects of the metallic additives. Topographical analysis showed that all deposited films exhibited uniform and smooth surfaces, consistent with high-quality $Bi_2Te_{2.7}Se_{0.3}$ growth, while compositional measurements confirmed that the metallic content remained at low levels. X-ray photoelectron spectroscopy verified that Cu and Ni preserved their elemental metallic states, with no detectable oxidation or telluride phase formation. Structural characterization using X-ray diffraction and Raman spectroscopy revealed no lattice distortion or secondary phases, indicating that the metallic species were mainly distributed along grain boundaries. By optimizing the Cu–Ni content through controlled PLD processing, a maximum room-temperature figure of merit (ZT) of 0.97 was achieved. This enhancement resulted from a combined increase in electrical power factor (2988 μW/m·K²) and a decrease in thermal conductivity to 0.93 W/m·K. The rise in the Seebeck coefficient is attributed to energy-selective carrier scattering at metal–semiconductor interfaces, underscoring the role of metallic nanoinclusions in advancing thermoelectric thin-film performance.

EES - D2 - P13

The influence of incorporating alkaline metals on alumina for xylitol hydrogenolysis over Ni catalysts

Vuyolwethu O. Ndabankulu[1], Alisa Govender[2], Holger B. Friedrich[1] and Mzamo L. Shozi[1]*
[1]University of KwaZulu-Natal, South Africa; [2]Durban University of Technology, South Africa

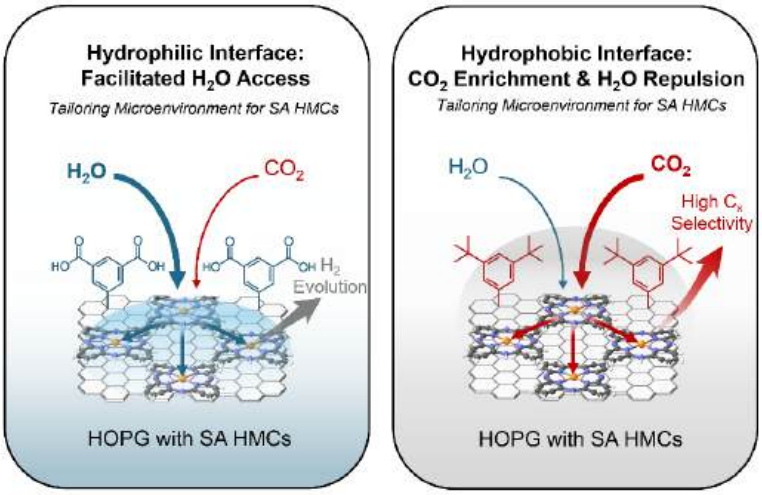
Bifunctional nickel catalysts Ni/MO-Al_2O_3 (M = Ba, Ca, Mg and La) were prepared by the co-precipitation method for the support, followed by wet impregnation of Ni and used for the hydrogenolysis of xylitol to glycols. According to the XRD data, the crystal structure of the support was maintained after loading Ni. All the prepared catalysts were mesoporous, as indicated by N_2 physisorption isotherms. XPS revealed Ni 2p peaks, which were assigned to NiO on the surface of the catalysts. The bifunctional catalysts exhibited good xylitol conversions and glycol selectivity over a 24-hour period. The surface structure suggests that Ni/BaO-Al_2O_3 (Ni/BA) promotes dehydrogenation and the retro-aldol reaction, which favours C2–C3 bond cleavage. The incorporation of alkaline metals reduced the formation of cracked products, such as methane and carbon dioxide, while increasing glycol yields. A combined yield of 80% to propylene glycol (PG) and ethylene glycol (EG) was thus obtained over Ni/BA at 200°C and a 40 bar H_2 pressure.

EES - D2 - P14

Tailoring the interfacial microenvironment: Hydrophilic/hydrophobic and cationic effects on CO2 reduction selectivity

Xingyu Li[1], Kunal Mali[1], Steven De Feyter[1]
[1]*Division of Molecular Imaging and Photonics, Dept. of Chemistry, KULeuven, Belgium*

Contemporary catalysis research seeks a rational correlation between atomic-scale structures and catalytic performance. For heterogeneous molecular catalysts (HMCs), the interfacial microenvironment—specifically the cationic effect within the electrochemical double layer—plays a pivotal role in governing activity and selectivity by stabilizing key intermediates through electrostatic interactions.[1] However, the effectiveness of these cations is heavily modulated by the local interface's chemical nature.



In this work, we regulate the local environment of HMCs by engineering vertical hydrophilic and hydrophobic interfaces on Highly Oriented Pyrolytic Graphite (HOPG) via molecular grafting, followed by the construction of self-assembled HMC networks. The morphology is characterized using STM, AFM, and Raman spectroscopy. Our results demonstrate that the hydrophilic interface facilitates H_2O access, promoting proton-coupled electron transfer and favoring the competing H_2 evolution reaction. Conversely, the hydrophobic interface creates a local microenvironment characterized by CO_2 enrichment and H_2O repulsion.[2] This spatial control not only suppresses HER but also optimizes the local cation distribution to stabilize CO_2 reduction intermediates, leading to high selectivity for carbon-based products (C_x).[3] This study offers fundamental insights into tailoring interfacial wettability and ion distribution to dictate CO_2RR selectivity.

Acknowledgements: Financial support from KU Leuven–Internal Funds (C14/23/090), FWO (G0A5U24N), and Chinese Scholarship Council (grant no. 202506050042) is acknowledged.

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EES - D2 - P16
3D laminated graphene photodetectors for non-contact monitoring of greenhouse gases

Hun-Seong Kim[1], Hyun Young Jung[1,2]
[1]Dept. of Energy System Engineering, Gyeongsang National University, South Korea; [2]Dept. of Energy Engineering, Gyeongsang National University, South Korea

Monitoring greenhouse gases (GHGs) is essential for effectively combating climate change. However, existing GHG detection systems are often costly, cumbersome, and sparsely deployed, limiting their ability to provide timely, localized data. Furthermore, current sensing technologies face challenges in indoor and densely populated environments due to limitations in detection mechanisms and constraints posed by physical setup or operating conditions. In this work, we present a novel photoelectric sensor based on three-dimensionally laminated graphene structures, engineered under high-temperature and high-pressure conditions to enhance light absorption through GHG layers. This configuration enables precise, non-contact detection of gas concentrations without requiring proximity between the gas and sensor. Our device demonstrated sensitivity to carbon dioxide at 216 ppm, carbon monoxide at 0.06 ppm, and a mixture of methane and carbon dioxide at 0.88 ppm. Notably, a significant photoresponse of 45% was observed under 12 μW/cm^2 of incident light in an environment containing 1.09 ppm of carbon monoxide. These findings lay the groundwork for scalable, low-cost GHG sensing platforms, paving the way for dense urban monitoring networks and smarter environmental management.

Acknowledgements: This research was supported from the Korean Meteorological Administration Research and Development Program (No. RS-2025-02316767).

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EES - D2 - P017

Continuous flow electrochemical oxidation of NaBr for the in-situ generation and telescoped utilisation of Br2

Davin Cronly[1], Megan Smyth[2], Scott Wharry[2], Tom Moody[2], Marcus Baumann[1]
[1]University College Dublin, Ireland; [2]Almac Sciences, UK

The synthesis of brominated compounds is of importance in the chemical industry for both final products and reactive intermediates in synthetic pathways.[1] However, the process often involves the use of toxic, and hazardous reagents. As such, the use of less hazardous and more easily handled brominating agents are looked to as a safer source of bromine for these reactions.[2] For this work we looked to develop a continuous flow methodology for the *in-situ* generation of Br_2 from sodium bromide. Utilising an electrochemical flow cell the bromide can be oxidised to give Br_2 which can be extracted to an organic solvent and separated using an inline liquid-liquid separator.
The developed method for generating Br_2 using a continuous electrochemical flow cell was telescoped to a range of continuous chemical reactions including photochemical benzylic brominations using a 365 nm LED lamp, the synthesis of esters and amides from a bromo acid intermediate, and the synthesis of carbamates from amides *via* a Hofmann reagent rection.

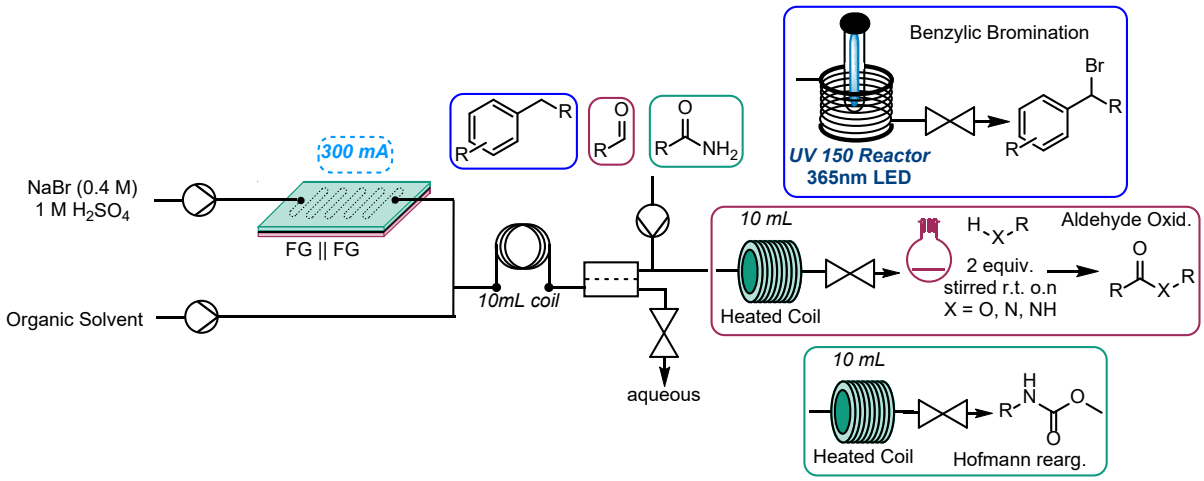

Fig. 1. Telescoped electrochemical Br2 generator and utilisations.

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EES - D2 - P18

A first principles study of heterostructure Ru/ClF for potential use as anode in Li ion batteries

Penny Govender[1], Krishna Govender[1], Francis Opoku[1,2], Blessing Masora[1]
[1]University of Johannesburg, South Africa; [2]KNUST, Ghana

The escalating demand for high-capacity energy storage has motivated the search for novel 2D anode materials for lithium-ion batteries (LIBs). Herein density functional theory investigates the RuClF/AlN heterostructure. ClRuF/AlN stacking (Stacking 2) was most stable, exhibiting a negative binding energy, with its dynamical stability confirmed by phonon calculations.
Electronic analysis reveals a reduced bandgap of 1.38 eV, suggesting enhanced conductivity compared to the individual monolayers. Lithium adsorption energy studies indicate strong ionic interactions, where interface storage is more energetically favourable than forming solid–electrolyte interphase species. A low measured diffusion barrier of 0.33 eV highlights the material's ability to facilitate rapid ion mobility.
This heterostructure achieves a high theoretical storage capacity of 564.29 mAh g^{-1}, significantly outperforming commercialised graphite. An average open-circuit voltage (OCV) of 0.78 V was obtained, falling within the ideal range for anode materials while effectively mitigating the risk of lithium dendrite growth. Multilayer configurations further enhance stability by buffering lithiation-induced strain, with volume expansion limited to 17–19%. AIMD simulations confirm the fully lithiated system remains thermally stable under operating conditions. These findings demonstrate that the RuClF/AlN heterostructure possesses the properties required for a high-performance, next-generation LIB anode material.

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EES - D2 - P19

Alkalinity-dependent structural features and Cr(VI) adsorption of one-pot synthesized Ca–Al layered double hydroxides

Lord Richard B. Verania[1], Joshua S. Geraldino[1], Sophia Isabel A. Alcabao[1], Ella A. Paraiso[1], Naomi Gabrielle M. Valenciano[1], Yasmin D.G. Edañol[1]
[1]Institute of Chemistry, University of the Philippines, Philippines

Hexavalent chromium (Cr(VI)) is a highly toxic and carcinogenic contaminant commonly released in industrial wastewater, posing severe risks to aquatic systems and agricultural productivity. In this study, Ca–Al layered double hydroxides (LDHs) were synthesized via a simple one-pot route using CaO and kaolin as low-cost solid precursors for Cr(VI) removal from water. The effect of the caustic solution-to-total solid precursor ratio (30:1 and 60:1, expressed as mL of alkaline solution per gram of CaO–kaolin mixture) on LDH formation and adsorption performance was systematically investigated. Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) confirmed the formation of Ca–Al LDH phases in both materials, with the 60:1 sample exhibiting more pronounced LDH features and improved structural ordering. Batch adsorption experiments, with residual dissolved chromium quantified by atomic absorption spectroscopy (AAS), showed that the 60:1 Ca–Al LDH achieved higher adsorption efficiency at lower initial Cr(VI) concentrations and an overall higher removal efficiency (≈70%) compared to the 30:1 sample (≈50%), which exhibited comparatively weaker uptake across the tested concentration range. This behavior suggests that increased alkalinity during synthesis promotes improved LDH development and a greater availability of active adsorption sites. Equilibrium adsorption data for both LDHs were best described by the Freundlich isotherm model, indicating heterogeneous surface adsorption and multilayer uptake of Cr(VI) ions. These results demonstrate that Ca–Al LDHs prepared from CaO and kaolin via a facile one-pot method are effective, low-cost adsorbents for Cr(VI) remediation in aqueous systems.

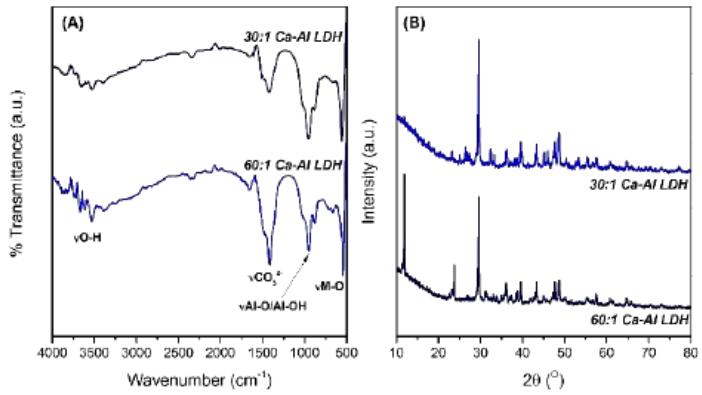

Fig. 1. (a) FTIR spectra and (b) powder X-ray diffraction (XRD) patterns of the Ca–Al hydroxide products

[1]Milagres, J. L.; et al. *J. Environ. Chem. Eng.* **2017,** *5*, 5469–5480.
[2]Edañol, Y. D. G.; et al. *Mater. Today Proc.* **2020**, *33*, 1809–1813.
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EES - D2 - P20

Repurposing a commercial plasma spraying torch: Quenching by turbulence, for efficient CO2 conversion

Helder Van Poyer[1], Ivan Tsonev[1], Yury Gorbanev[1], Matthias Albrechts[1], Hugo Vallet[1], Annemie Bogaerts[1]

[1]Research Group PLASMANT and Center of Excellence PLASMA, Electrification institute, University of Antwerp, Belgium

Reducing greenhouse gas concentrations, such as CO_2, is a major scientific challenge today. Atmospheric-pressure plasma-based CO_2 conversion offers a promising route to convert CO_2 into CO, a key chemical feedstock.[1, 2] For industrial use, lab-scale plasma reactors must be upscaled to achieve higher throughput. Repurposing already developed technologies, like plasma spraying reactors, for gas conversion could offer an efficient and faster route toward industrially viable scale-up.

We investigated CO_2 conversion in a commercially available plasma spraying torch, in a wide range of flow rate and input power. We studied conversion, energy efficiency and afterglow temperatures, obtaining a maximum conversion of ca. 19% (at specific energy input (SEI) of 255 kJ mol^{-1}) and a maximum energy efficiency of 34% (at SEI of 61 kJ mol^{-1}), on par or better than most literature reports. .[3-10] Importantly, this is reached without additional thermal quenching in the afterglow to avoid backreactions, which is typically needed for efficient conversion in literature.

To better understand the experimental results, we developed a novel, fully coupled magnetohydrodynamic thermochemical model, describing turbulent flow, heat transfer, transport of species and chemistry, as well as the electric and magnetic fields in the CO_2 plasma arc reactor. The model is validated against the experiments in terms of conversion, energy efficiency and afterglow temperatures. The good agreement with experimental data demonstrates that our 2D axisymmetric stationary model approximations can provide a reasonable description of our plasma torch. Most importantly, our model explains how reactor design can prevent back reactions effectively by turbulent quenching of the effluent.

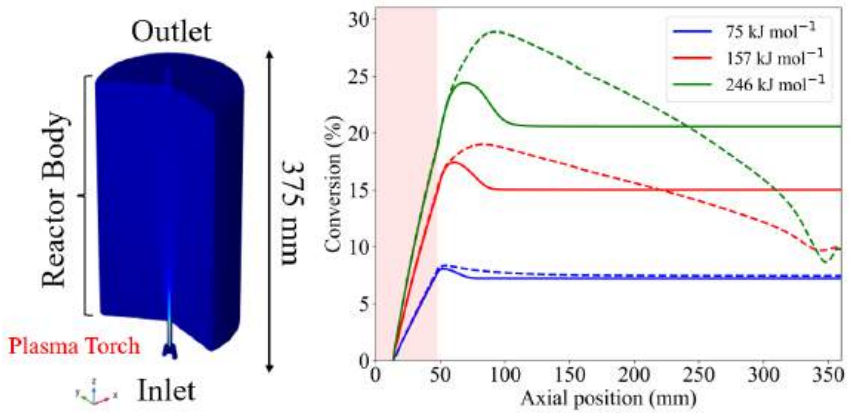

Fig. 1. Graphical representation of the plasma torch and the reactor chamber (left) with the calculated conversion as a function of axial position, for three different SEI values, with (solid) and without (dashed) turbulent quenching, for 10 slm flow rate (right). The plasma region is indicated in red.

Turbulent quenching resulting in higher conversion at the end of the reactor, especially at high SEI values, as can be seen in Figure 1. Combined with the fact that this plasma torch operates at higher power and flow rate than typical lab-scale plasmas, this natural quenching makes this plasma torch of great interest for industrial-scale gas conversion applications.

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[2]Snoeckx, R.; Bogaerts, A. Plasma technology – a novel solution for CO2 conversion? *Chemical Society Reviews* **2017**, *46* (19), 5805-5863, 10.1039/C6CS00066E.
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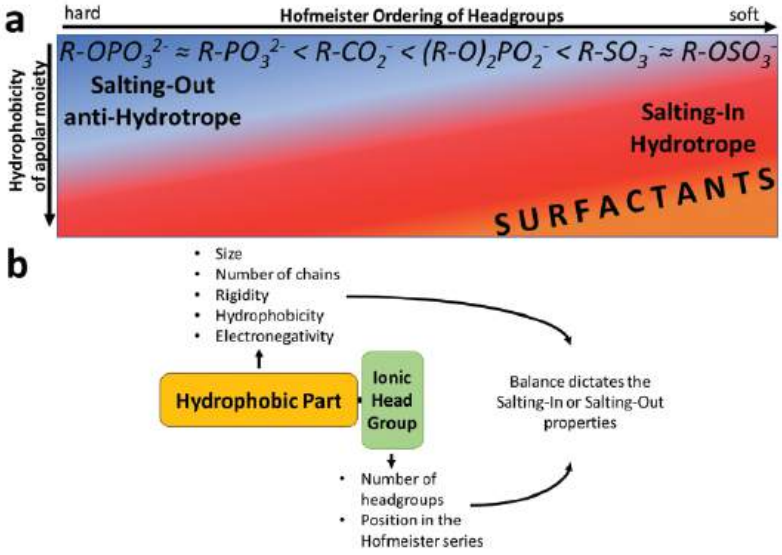
[10]O'Modhrain, C.; Trenchev, G.; Gorbanev, Y.; Bogaerts, A. Upscaling Plasma-Based CO2 Conversion: Case Study of a Multi-Reactor Gliding Arc Plasmatron. *ACS Engineering Au* **2024**, *4* (3), 333-344.

EES - D2 - P21
Strategies for environmentally friendly solvent media

Werner Kunz[1], Eva Mueller[1], Didier Touraud[1]
[1]University of Regensburg, Institute of Physical and Theoretical Chemistry, Germany

The first example concerns the optimization of medium structuring to improve organic reactions. Especially, I will discuss in how far surfactants or other, milder structuring additives are necessary or useful to this purpose[1].
In a second example, I will show how natural polyphenols can not only play the role of valuable antioxidants, but even may help increase the solubility of other valuable plant extracts in water. This can be useful to optimize extraction processes and even green formulations of food and cosmetic additives[2,3].
Third; I will show how the old Hofmeister concept can be extended to range now from strong salting-out compounds via salting-in, hydrotropes until surfactants[4]:



And finally, I will put together most relevant strategies to increase the solubility of a component in a desired, if possible “green” solvent[5].

[1]Hofmann, E. et al., *Chem. Eng. J*. **2023**, *472*, 144599-607. Giedyk, M. et al. *Nat. Catal.* **2020**, *3*, 40-47.
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[3]Ulmann, N. et al., *J. Coll. Interf. Sci.*. **2023**, *641*, 631-642.
[4]Mehringer, J. et al., *Phys. Chem. Chem.Phys.* **2021**, *23*, 1381-91.
[5]Müller, E., Kunz, W. *Chem.Sus.Chem.* **to appear.**

EES - D2 - P22

Plasma-based CO_2 conversion: Scaling from lab to industry towards continuous CO production

Robbe Bryssinck[1,2,3], Annemie Bogaerts[1], Tom Van Assche[2], Georgi Trenchev[3]
[1]Research group PLASMANT, Center of Excellence PLASMA, and Electrification Institute, University of Antwerp, Belgium; [2]Vrije Universiteit Brussel, Belgium; [3]D-CRBN, Belgium

The last decade(s) showcased the potential of plasma-based CO_2 conversion in a lab-scale environment[1, 2]. However, transitioning from lab-scale to an industrial setting is necessary to validate the technology and anchor its place in the industrial landscape. Additionally, the post-plasma effluent stream needs to be purified to ensure a pure CO stream to an industrial off-taker. Several technologies exist to perform this purification, for example pressure swing adsorption (PSA).
In this work, several carbon sources (activated carbon, biochar, industrial waste) were tested to investigate the influence of their origin on the reactor performance. The results showed that the origin negligibly influences performance in terms of CO vol.% (see Figure 1). However, each carbon type has a different consumption rate and operational lifetime, an important factor for industrial feasibility. Furthermore, experiments were performed on a pilot scale reactor containing seven gliding arc plasmas in parallel. The results (also in Figure 1) showed an increase in CO concentration from 52 vol.% to 68 vol.% and a decrease in energy cost from 4.1 kWh kg_{CO}^{-1} to 1.8 kWh kg_{CO}^{-1} compared to the lab setup, thus proving its feasibility. Nonetheless, the mixture still contains CO and unconverted CO_2, while industrial partners require a >98.5 vol.% CO stream for synthesis processes. Therefore, a suitable separation method needs to be determined. An adsorptive separation method, namely PSA, was chosen as the most promising technology. Several adsorbents were screened by measuring pure component isotherms and dynamic breakthrough curves. As a result, adsorbent capacities and selectivities were determined, which can be used in a model to predict CO purity and recovery.

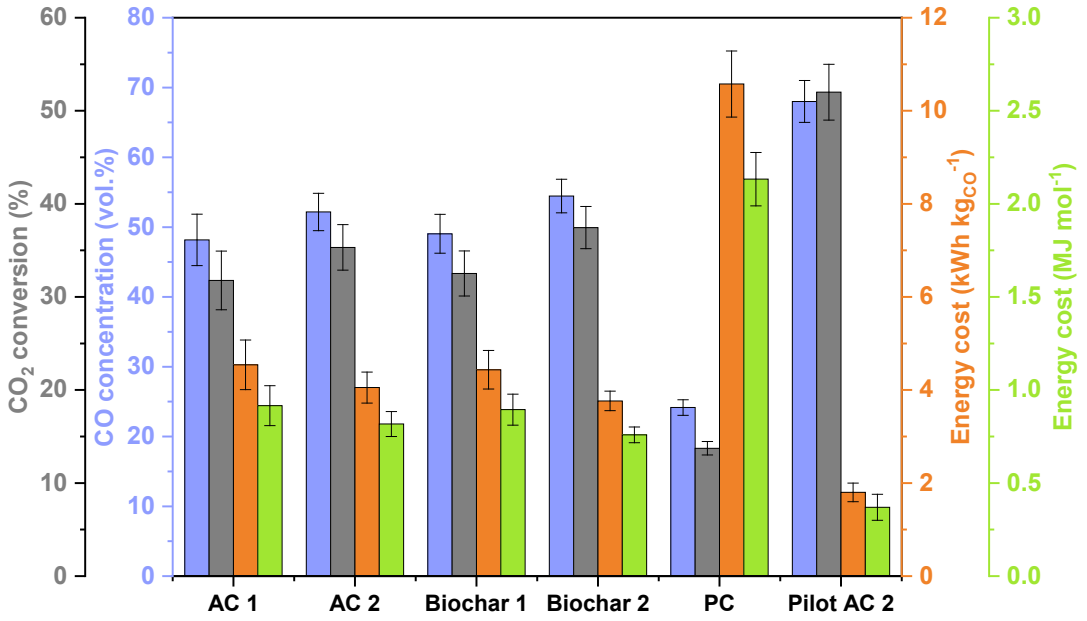

Fig. 1. CO concentration (vol.%, blue), CO_2 conversion (%, grey), energy cost (kWh kg_{CO}^{-1}, orange), and energy cost (MJ mol^{-1}, green) for three different carbon types (activated carbon: AC1 and AC2; biochar (1 and 2) and pyrolytic carbon, PC) tested on lab-scale and also AC2 on pilot scale.

[1]Snoeckx, R.; Bogaerts, A. Plasma technology–a novel solution for CO 2 conversion? *Chemical Society Reviews* **2017**, *46* (19), 5805-5863.
[2]Bogaerts, A. Plasma technology for the electrification of chemical reactions. *Nature Chemical Engineering* **2025**, 1-5.

EES - D2 - P23

Highly dispersed Cu on CeO_2-Al_2O_3 via a novel synthesis route for efficient selective hydrogenation of HMF

Lole Jurado[1], Natalia Victoria Paniagua[1], Irene Malpartida[2] and Pedro Maireles Torres[1]
[1]Dept. of Inorganic Chemistry, Crystallography and Mineralogy, Faculty of Sciences, University of Malaga, Spain; [2]Deasyl Company, Les-Ouates, Switzerland

Single-atom catalysts (SACs) maximize metal atom utilization and offer unique reactivity.[1] Wetness impregnation is the most common method due to its simplicity and scalability; however, it often leads to aggregation during drying or calcination.[2] This limits the efficiency and selectivity of SACs. **Mechanosynthesis** provides an energy efficient method, ensuring intimate mixing of metal precursors and support, strengthens metal–support interactions, and reduces metal migration during activation or reaction.[3]
This study evaluates the influence of preparation method on Cu dispersion over CeO_2-Al_2O_3 and its impact on HMF hydrogenation. Wetness impregnation (Cu) is compared with mechanosynthesis (Cu*) to identify the most effective route for stabilizing active sites and enhancing catalytic performance.

Table 1 shows the physico-chemical properties of as-prepared materials. Mechanosynthesis improves Cu catalyst characteristics compared to wet impregnation. The Cu* catalyst has higher specific surface area than Cu one (195 vs 175 m^2/g), enhancing dispersion as indicates CO chemisorption (29 vs 27 m^2/g). Bulk Cu content is similar (0.6 wt%), but surface Cu concentration differs, since impregnated Cu shows 1.6 wt%, while this is undetectable in Cu*, suggesting atomic-level dispersion or embedding in the support. HAADF-TEM (**Figure 1.a-b**) confirms highly dispersed Cu atoms in both catalysts. Catalytic performance of both materials was evaluated in HMF hydrogenation at 120 ºC and 30 bar of H_2.

Table 1. Physico-chemical properties of catalysts prepared by impregnation (Cu) and mechanosynthesis (Cu*)

	$D_{support}$ (nm)	SSA (m^2/g)	Bulk Cu content (wt%)[a]	Surface Cu content (wt%)[b]	Cu dispersion (m^2/g of metal)[c]
CeO_2-Al_2O_3	49	154	-	-	-
Cu	50	175	0.54	1.6	27
Cu*	47	195	0.57	N.D	29

[a]Measured by ICP-OES
[b]Calculated from XPS of fresh materials
[c]Calculated from CO chemisorption after pre-reduction at 600 ºC in H_2 atmosphere

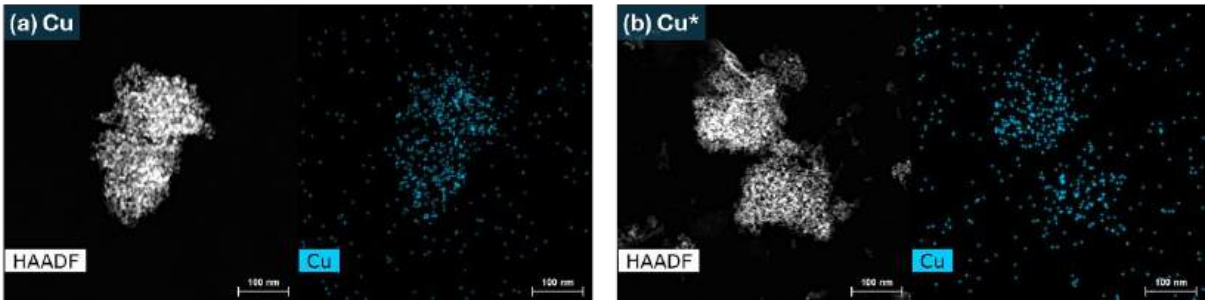

Fig. 1. HAADF-TEM and elemental mapping of catalyst prepared by **(a)** impregnation (Cu) and **(b)** mechanosynthesis (Cu*)

This work was funded by the European Union under the Marie Sklodowska-Curie grant agreement No. 101106349.

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EES - D2 - P24
Fouling-resistant metal-organic framework monoliths for pharmaceutical water treatment

Renz Marion G. Garcia[1], Khianne Ed Miguel Orteza[1], Zhang Liu[2], King Lun Yeung[1,2]
[1]Dept. of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, China; [2]Division of Environment and Sustainability, The Hong Kong University of Science and Technology, China

Metal-organic frameworks (MOFs) demonstrate exceptional capacities for pharmaceutical removal. However, practical deployment in water treatment remains limited by powder handling difficulties, particle release and recyclability concerns, and performance degradation from fouling by natural organic matter (NOM). Here, we demonstrate that a facile fabrication approach transforming MOF powders into centimeter-scale monolithic beads with high MOF loading (>60 wt. %) can maintain high ciprofloxacin (CIP) adsorption capacity and robust fouling resistance even in the composite form. Metal center chemistry emerges as a critical determinant of fouling resistance even after transforming MOF powders to monoliths. Systematic investigation compared zeolitic imidazolate frameworks with Zn (ZIF-8) or Co (ZIF-67) metal centers. Both MOF types were incorporated into alginate matrices with or without crosslinked poly(sodium 4-styrenesulfonate) (PSS). The results demonstrate that metal center identity governs composite fouling behavior in humic acid (HA)-containing water. Despite identical imidazolate ligands, matching alginate matrices, and similar baseline CIP capacities (33-39 mg g^{-1}), ZIF-8/alginate composites showed significant fouling with 73.2% CIP capacity retention after sequential HA exposure, while ZIF-67/alginate composites maintained 107.6% retention. Addition of PSS crosslinked network substantially improved ZIF-8 performance to 94.0% retention, representing a twenty-one percentage point increase. This comparison demonstrates that appropriately selected polymer matrices can overcome unfavorable surface chemistry to achieve comparable performance across different metal centers. Counterintuitively, results showed that HA binding capacity of MOF powders does not predict composite fouling behavior. Furthermore, MOF adsorption sites remained accessible even when incorporated in a dual-polymer matrix. Surface characterization through Fourier-transform infrared spectroscopy, x-ray photoelectron spectroscopy, and zeta potential measurements were performed to explain these performance differences. This composite formulation and monolith fabrication method simultaneously addressed powder handling challenges and fouling resistance, enabling practical deployment of promising MOF powders into large-scale water treatment systems.

Keywords: Metal-organic frameworks, fouling, water treatment

EES - D2 - P25
Carbon nitride allotropes for photo(electro)catalytic reactions

Sue-Faye Ng[1]
[1]Max Planck Institute of Colloids and Interfaces, Germany

Solar-driven catalytic reactions are a sustainable method to turn waste to value-added by product. This work will showcase the use of graphitic carbon nitrides for photo and electro-driven catalytic reactions, without the use of precious metal cocatalysts.[1,2] Herein, we introduce a strategic approach for functionalizing poly(heptazine imide) with triazole groups via a one-step calcination process using alkali-metal salts (NaCl/KCl/LiCl). This allotrope of carbon nitride could effectively promote solar-driven hydrogen peroxide and benzaldehyde production as well as CO_2 reduction. Additionally, the catalyst was also active towards the electrocatalytic reduction of various organic compounds. This work explores the effect of alkali salt melts and carbon nitride precursors on the material properties, and subsequently, the photo(electro)chemical performance of the catalyst. The future direction of the research will also include different modification methods as well as potential scale-up considerations.

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EES - D2 - P026

Effect of Ni loading and Fe promotion in NiFe–N–C catalysts for CO_2 electrolysis

Oriana Calderón Leal[1], Laura Fuentes Rodriguez[1], Mariia Galaburda[2]*, Bahareh Khezri[1,3,4]*
[1]Dept. de Química Física i Inorgànica, Universitat Rovira i Virgili, Spain; [2]Chuiko Institute of Surface Chemistry, Ukraine; [3]Catalan Institute for Research and Advanced Studies (ICREA), Barcelona, Spain; [4]Institute of Chemical Research of Catalonia (ICIQ-CERCA), The Barcelona Institute of Science and Technology (BIST), Spain

Electrochemical CO_2 reduction (CO_2RR) to CO is an attractive route to store renewable electricity in a transportable C_1 feedstock, but catalyst design must couple efficient CO_2 activation with suppression of the competing hydrogen evolution reaction (HER). Here we investigate Ni–Fe–N-doped carbon catalysts (NiFe–N–C) consisting of nitrogen-containing carbons with tunable metallic Ni content (10–60 wt%) and iron doping fixed at 5 wt% of the Ni content. The carbon framework (amorphous graphitic carbon nitride (g-C_3N_4-like), graphitic carbon, and/or carbon nanotubes) provides a platform to tune conductivity, nitrogen speciation, and metal–support interactions.

NiFe–N–C materials are synthesized by integrating N-rich carbon precursors with Ni and Fe sources, followed by controlled thermal treatment to generate dispersed metal nanoparticles and possible M–N (M = Ni, Fe) coordination environments embedded in the N-doped carbon matrix. Phase composition, carbon ordering, porosity, and metal dispersion/speciation assessed by XRD, Raman spectroscopy, N2 sorption, electron microscopy, and XPS/ICP analysis. CO2RR performance evaluated in CO_2-saturated aqueous electrolyte using three-electrode configurations, while gaseous products are quantified by gas chromatography to determine CO selectivity and CO/H_2 production rates.

Here we test whether lower overall metal loadings yield smaller, less agglomerated nanoparticles and increase access to catalytically relevant sites. We further examine Fe as a promoter for CO_2 binding and activation, with the expectation that Fe incorporation shifts selectivity toward CO over HER. Preliminary screening indicates that Ni-containing catalysts outperform metal-free N-carbons for CO production, and that Fe co-doping can further suppress H_2 formation under comparable conditions. Ongoing work correlates selectivity trends with Ni loading, carbon phase, and nitrogen/metal speciation to establish structure–activity descriptors and guide metal-lean NiFe–N–C catalysts for efficient CO_2-to-CO electrolysis. These insights will inform rational design of durable, selective carbon–metal composites enabling stable, practical CO_2-to-CO electrolysis.

EES - D2 - P027
Recyclable plastics from bio-based monomers

Lutz Burow[1], David Malsbenden[2], Alexander Hoffmann[1], Dominik Wöll[2], Sonja Herres-Pawlis[1]
[1]Institute of Inorganic Chemistry RWTH Aachen University, Germany; [2]Institute of Physical Chemistry RWTH Aachen University, Germany

In the midst of dwindling fossil resources and the highest ocean pollution, new polymers need to be developed from bio-based feedstocks with a clear end of live plan in mind. Monomers like α-ketoglutaric acid and 2,3-butanediol make such polyesters possible by using fermentation of biomass instead of crude oil as the resource.[1,2] As end-of-life options, polyesters feature breaking points in form of ester moieties for chemical recycling and the chance of biodegradability. Moreover, the monomers are non-toxic towards the human organism.
Through polycondensation, α-ketoglutaric acid and 2,3-butanediol were polymerised with a suite of comonomers to form tailored polyesters depending on the catalyst used. The combination of acid and keto moieties in the monomer leads to branching during the polycondensation yielding unique viscoelastic properties.
A variety of polycondensation catalysts already established in the industry were compared with highly active metal guanidine catalysts. To compare, the conversion needed to be tracked accurately. This was facilitated by different end-group analytics, like phosphitylation of hydroxyl moieties as well as single molecule tracking to compare branching. Additionally, macroscopic methods like GPC, DSC, TGA and rheology were used to establish structure property correlations.
Rheology was the most important method for analysing the unique viscoelastic properties of polyesters containing α-ketoglutaric acid. Using time-temperature superposition, branching of the monomer was analysed at different conversion time and with different comonomers to yield a novel thermoset polyester.
In summary, the poster features a suit of novel, bio-based polyesters applicable as thermosets in adhesive formulations.

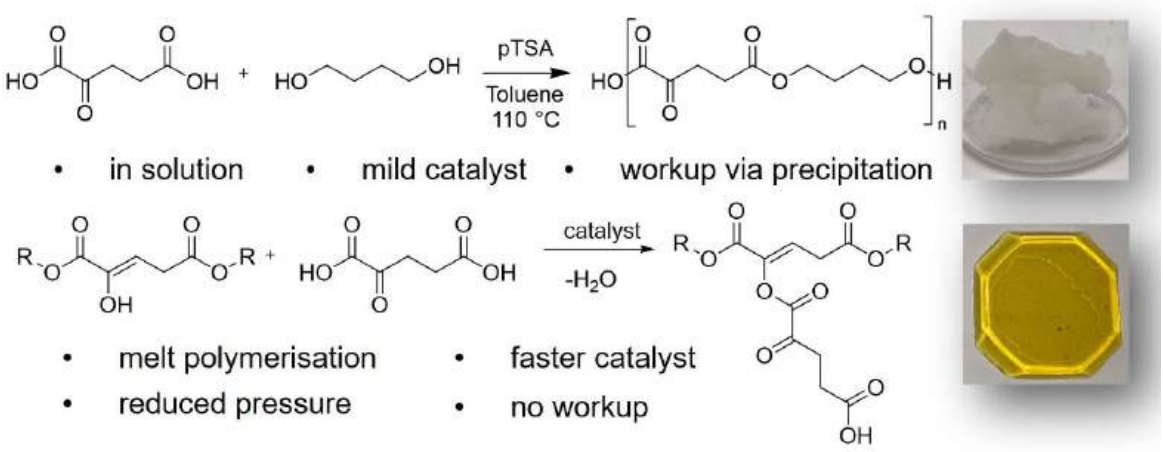

Fig. 1. Comparison between linear and branched polymerisation of α-ketoglutaric acid.

[1]L. Halle, D. Höppner, M. Doser, C. Brüsseler, J. Gätgens, N. Conen, A. Jupke, J. Marienhagen, S. Noack, Bioresour. Technol. 2025, 416, 131803.
[2]D. G. Barrett, W. Luo, M. N. Yousaf, J. Mater. *Chem. B* **2015**, *3*, 1405-1414

EES - D2 - P28

A water-based synthetic route to the metal-organic framework UiO-66 starting from PET derived terephthalate esters

Pietro Agola[1], Marco Taddei[1,2]

[1]University of Pisa, Dept. of Chemistry and Industrial Chemistry, Italy; [2]National Interuniversity Consortium of Materials Science and Technology, Italy

The benchmark Zr-terephthalate MOF UiO-66 is typically prepared and purified using *N*,*N*-dimethylformamide (DMF)[1] because of the limited solubility of terephthalic acid in the most common organic solvents and in water. The use of DMF is one of the major drawbacks for the transfer of UiO-66 in applications since DMF is flammable, toxic and teratogenic, to the point that its industrial use is restricted in the EU.[2] The development of a DMF-free process to produce UiO-66 is a topic of interest to enable commercial deployment of this MOF.

We developed a water-based route to synthesise UiO-66 through the in situ formation of the linker by hydrolysis of the esters dimethylterephthalate and bis(2-hydroxyethyl)terephthalate, obtainable from the chemical recycling of waste polyethyleneterephthalate (Figure 1). Hydrochloric acid and acetic acid were used as modulators during the synthesis to control the kinetics of ester hydrolysis and MOF crystallisation, aiming to avoid collateral precipitation of terephthalic acid. A design of experiments was employed to optimise the reaction parameters, finding that 15 molar equivalents of hydrochloric acid enable ester hydrolysis without inhibiting crystallisation, while acetic acid controls which crystalline phase is obtained, favouring the desired product at 15 molar equivalents. The optimised conditions afford UiO-66 with high crystallinity and porosity in just 2 hours at 90 °C. We also developed a DMF-free workup protocol based on the use of an ethanol/dimethylsulfoxide mixture and water. 50-fold scale-up was demonstrated using a round bottom flask, producing UiO-66 with properties comparable to the product of the small-scale synthesis and with a space-time yield > 200 kg m^{-3} d^{-1}.[3]

Figure 1. Water-based Synthesis of UiO-66 starting from terephthalate esters as the source of linker.

Funding: This work was supported by the European Innovation Council Pathfinder project *DAM4CO2* (n. 101115488).

[1]J. Winarta, *et al. Cryst. Growth Des.* **2020**, *20*, 1347–1362

[2]https://eur-lex.europa.eu/eli/reg/2021/2030

[3]P. Agola, M. Taddei *RSC Sustainability* **2026**, *4*, 466-476

EES - D2 - P29
Electrical characterization of a microbially produced, highly conductive MOF material

Daniel Modafferi[1], Cosimo Tommasi[2], Silvia Hidalgo-Martinez[1], Herre van der Zant[2], Filip Meysman[1]
[1]University Antwerp, Belgium; [2]Delft University, The Netherlands

Conventional flexible electronics made from metals or synthetic polymers generally have a large carbon footprint, contain toxic components and are difficult to recycle. Achieving sustainability and circularity in electronics represents hence a grand social challenge. Biomaterials could inspire green synthetic and engineering routes for electronic materials, but the low conductivity of known biomaterials presents an important fundamental roadblock.
A recent discovery shows that certain bacteria (called cable bacteria) can produce highly conductive wires, which are a million-fold more conductive than known biomaterials. These fibers are highly flexible, stretch for centimeters long and reach an astonishingly high electric conductivity of >100 S/cm, which is comparable or even better than synthetic conductive polymers. Recently, it was demonstrated that these highly conductive fibers contain a bundle of nanoribbons that each consist of a one-dimensional metal organic framework (MOF). This unique chemical structure enables the material to be highly conductive.
This biologically produced MOF-material provides a novel and promising pathway for sustainable production of bio-based electronic materials. Here, we report on the detailed electrical characterization of the material. This provides insight into the unique charge transport mechanism implicated, and illustrates the competitiveness of the material compared to current solutions in flexible printed electronics (e.g. metal-based inks).

EES - D2 - P30
Ni-based catalyst deactivation in the dry reforming of HDPE pyrolysis volatiles

Leire Olazar[1], Miren Ugarriza[1], Katrin Santin[1], Laura Santamaria[1], Stephanie Arias[1], Gartzen Lopez[1,2], Maite Artetxe[1]
[1]University of the Basque Country (EHU), Spain; [2]IKERBASQUE Basque Foundation for Science, Spain

An enormous amount of plastic is produced each year, with a great portion not being recycled and ultimately ending up in landfills or being incinerated. Moreover, chemical and energy industries are still heavily dependent on fossil resources, which are unsustainable and major contributors to greenhouse gas emissions and global climate change [1]. Through thermal decomposition of plastic wastes followed by catalytic conversion with CO_2, volatiles are converted into syngas, which is a versatile mixture of hydrogen and carbon monoxide with applications in energy generation and chemical synthesis [2].
The feasibility of any large-scale catalytic process relies on the development of suitable catalysts, with the main challenge being the prevention of catalyst deactivation. Therefore, delving into the knowledge of the understanding of the main mechanisms responsible for catalytic activity loss is of uttermost importance. Different Ni based catalysts supported on Al_2O_3 and MgO were prepared and tested. Moreover, the incorporation of La_2O_3 as promoter was also evaluated. Finally, the performance of these custom prepared catalysts was compared to the one attained with a commercial Ni/Al_2O_3 catalyst.
The commercial Ni/Al_2O_3 catalyst showed the highest initial activity but poor stability due to the high coke deposition rate and remarkable Ni crystallite sintering. Although the Ni/La_2O_3-Al_2O_3 initial activity was not very high, it showed a positive performance in terms of stability. This is due to the basic nature of the La_2O_3 promoter, which enhances the adsorption of CO_2 on basic surface sites and promotes coke gasification, thereby preventing catalyst deactivation. The Ni/MgO catalyst proved to be of limited interest for the dry reforming of HDPE pyrolysis volatiles in terms of both activity and stability.

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EES - D2 - P31

Efficient and sustainable production of calcium carbonate from oyster shell waste: A carboxylic acid-mediated green processing approach

Jin Hyng Lee[1], Sang Heon Lee[1], Ji Yeon Park[1], Byoung Seung Jeon[1], and Hye Sun Lee[1]
[1]Korea Institute of Ceramic Engineering and Technology, Rep. Korea

The accumulation of massive oyster shell waste poses a significant environmental challenge for coastal industries. However, with a calcium content of approximately 94.7%, these shells represent a valuable yet underutilized biogenic source for high-purity precipitated calcium carbonate (PCC). This study proposes a sustainable valorization strategy by replacing conventional hydrochloric acid (HCl) with environmentally benign carboxylic acids—acetic, formic, and citric acid—for calcium extraction and subsequent PCC synthesis.Our results demonstrate that carboxylic acids are highly effective as leaching agents. High-purity PCC (>98% Ca) was successfully synthesized, with calcium recovery efficiency being strongly dependent on the acid type and concentration. Notably, citric acid achieved a maximum recovery of 98.7% at 1.5 M, while formic and acetic acids reached 92.3% and ~80% at 2.0 M, respectively, showing performance comparable to mineral acids.A key finding of this research is the superior phase control offered by organic acids. Unlike HCl, which exclusively yields stable calcite, acetic and formic acids facilitated the formation of metastable polymorphs, such as vaterite and aragonite, at lower concentrations (≤1.0 M). Conversely, high concentrations of citric acid favored the formation of calcium citrate complexes. These phase transitions are governed by the acid-mediated distribution of ionic species (Ca^{2+}, CO_3^{2-}, COO^-), where carboxyl functional groups act as molecular templates modulating nucleation and crystal growth. These findings provide critical mechanistic insights into tunable PCC crystallization and highlight carboxylic acids as green, efficient agents for transforming marine waste into high-value functional materials, directly contributing to the circular economy in the chemical industry.

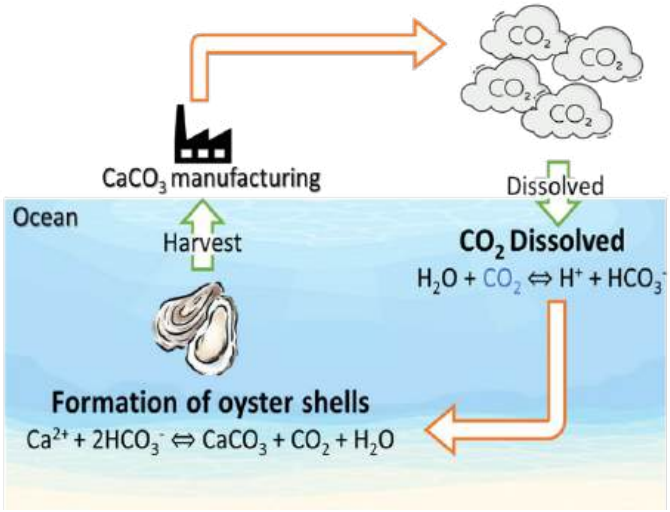
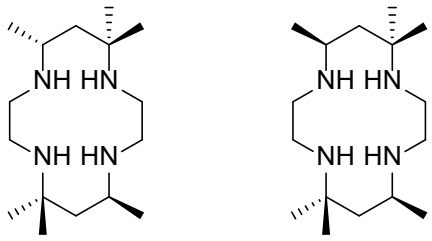


Fig. 2. Circular economy framework of oyster shell waste: Integrating natural biomineralization with sustainable valorization processes

EES - D2 - P32
Reactivity of dioxygen and hydrogen peroxide with macrocyclic iron complexes

Kevin Keller[1], Siegfried Schindler[1]
[1]Institute of Inorganic and Analytical Chemistry, Germany

Oxygenation reactions play an important role in the chemical industry. Every year, large quantities of products are manufactured through such processes. For example, adipic acid is obtained through several steps from the oxygenation of cyclohexane. From a sustainability perspective, most of the industrial syntheses are far from ideal. To develop more sustainable methods, modelling the active site of metallo enzymes, which carry out oxidation reactions via reactive oxygen intermediates, is promising. These intermediates often involve iron–oxo species. Several research groups, have succeeded in synthesizing mononuclear iron–oxido species using strong oxidants together with the TMC (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane) ligand.[1,2] More recently, Ray[3] and co-workers demonstrated with cyclam complexes that this can also be achieved using cyclam and molecular oxygen as the oxidant. This raises the question of how other cyclam derivatives behave under similar conditions, particularly when they are chiral. Since our research group has previously gained experience using tet a/b as ligands in oxygen activation with copper, this project presents the corresponding results obtained from experiments on the analogous iron complexes.[4]



tet a tet b

Fig. 1. Molecular structure of rac-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane (tet a and tet b)

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EES - D2 - P33

Diverse recycling pathways of graphitic anode materials for advancing sustainable battery technology

Rocco Cancelliere[1], Chiara Marcatili Bevini[1,2], Myriam D'Alù[1,2], Annalisa Aurora[1], Emanuele Serra[1], Pier Paolo Prosini[1], Laura Silvestri[1]

[1]Dept. of Energy Technologies and Renewable Sources, ENEA C.R. Casaccia, Italy; [2]Dept. of Chemistry, University Sapienza of Rome, Italy

Climate change poses a significant barrier to achieving sustainable development goals (SDGs).[1] Accelerating the transition to clean energy, with lithium-ion batteries (LIBs) as a cornerstone, is critical.[2] LIBs dominate electrified mobility and energy storage, especially in the rapidly growing electric vehicle (EV) market, where global sales rose from 0.7 million in 2015 to 10 million in 2022 and are expected to reach 30 million by 2030.[3] However, scaling up LIB production to meet this growing demand exposes critical challenges, including reliance on scarce raw materials, high production costs, and safety concerns.[4] Each EV battery pack requires approximately 8 kg of lithium, equating to a demand of 240 million tons to meet future EV targets.[5] With global lithium reserves estimated at 20 million tonnes, factors like limited production feasibility and purity constraints intensify resource pressures, particularly as lithium is vital for other applications.[6] Consequently, effective management of retired batteries is essential to avoid environmental pollution, resource depletion, and supply chain risks.[5,6] Reuse and recycling of these batteries are critical solutions endorsed by the scientific and industrial sectors. Conventional recycling techniques, primarily pyrometallurgical and hydrometallurgical methods, have demonstrated limitations, including high energy demands, chemical waste production, and incomplete material recovery.[6,7] To address these challenges, diverse recycling pathways are being explored, aiming to improve resource efficiency, minimize environmental impact, and contribute to a circular economy for LIBs.[8] This presentation will explore innovative recycling strategies, including direct recycling, with a detailed chemical-physical characterization of the recovered materials. It will also highlight their potential applications in developing more sustainable electrode materials, along with insights into their preliminary electrochemical performance when incorporated into LIBs.

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EES - D2 - P34

Valorisation of HDPE by pyrolysis and in-line catalytic cracking with metal-modified ZSM5 zeolite

Katrin Santin[1], Stephanie Arias[1], Miren Ugarriza[1], Daniel Goma[1], Pablo Comendador[1], Maider Amutio[1], Maite Artetxe[1]

[1]University of the Basque Country (UPV/EHU), Spain

Plastics have become an essential product of the current lifestyle, because of their excellent properties and versatility. Consequently, annual plastic waste world generation has increased and will continue to increase in the future. For this reason, the management or recovery of this waste is indispensable. Chemical recycling, and especially catalytic pyrolysis, is a promising option to recover high value-added products from plastics. The use of catalyst is necessary to increase the selectivity of these products, and ZSM5 zeolite has demonstrated a great selectivity to olefins and aromatics. In addition, the modification of zeolite through the addition of metal can enhance catalyst selectivity [1,2,3].

In this work, four synthesized catalysts have been tested in the pyrolysis and in-line catalytic cracking of HDPE. The zeolites (ZSM5) were impregnated with different metals (Ni, Fe, Zn, Zr) and they were agglomerated with alumina and bentonite. The plastics pyrolysis step (500 ºC) has been carried out in a conical spouted bed reactor, and the volatile stream has been fed in line to a fixed bed catalytic reactor (550 ºC, 15 $g_{catalyst}$ min $g_{plastic}$).

The experimental results showed in Figure 1 reveal that Ni has a great impact on product distribution, reducing the light olefins yields while increasing that of BTX. In contrast, Fe and Zr do not show a significant effect.

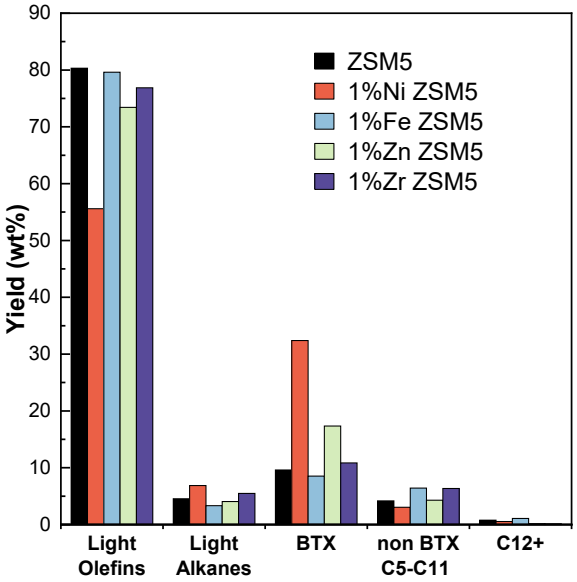

Fig. 1. Effect of metal modification over product distribution the pyrolysis and in-line catalytic cracking of HDPE.

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EES - D2 - P35

Thermodynamic assessment of the joint valorization of CO_2 and waste plastics by pyrolysis and in line combined reforming for syngas production

Miren Ugarriza[1], Leire Olazar[1], Farid Atashi[1], Pablo Comendador[1], Katrin Santin[1], Gartzen Lopez[1,2], Maite Artetxe[1]

[1]Dept. of Chemical Engineering (UPV/EHU), Spain; [2]IKERBASQUE Basque Foundation for Science, Spain

Plastic waste mismanagement and CO_2 emissions are critical environmental concerns. The joint valorization of both pollutants can be achieved through the pyrolysis of plastic waste in a conical spouted bed reactor and in-line dry steam reforming to produce synthesis gas [1,2].

In this work, the influence of the operating conditions of the second stage is analysed through the thermodynamic equilibrium simulation, with the aim of establishing the best conditions to obtain a high-quality syngas together with the highest possible CO_2 conversion. The study establishes the influence of temperature (600-800 ºC), the ratio between the reforming agents and the amount of the carbon fed (1-2), and the ratio between the reforming agents (0.5-2) on the H_2/CO ratio of the syngas and on the CO_2 conversion during the reforming of the high-density polyethylene volatiles of pyrolysis. It also determines the effect of feed composition on the H_2/CO ratio and the conversion of CO_2.

The results indicate that increasing the temperature favours both steam and dry reforming, while the reverse Water Gas Shift reaction has negligible influence. Increasing the ratio between the reforming agents and the amount of carbon fed and the steam/CO_2 ratio enhances steam reforming but hinders dry reforming, resulting in a higher H_2/CO ratio but a lower CO_2 conversion. These results highlight that a compromise between the operating parameters needs to be established to adjust the H_2/CO ratio while obtaining the highest CO_2 conversion possible. Feeding different plastics demonstrates the high potential of polyolefins and polystyrene to produce syngas, while polyethylene terephthalate proves to be the most difficult polymer to reform.

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EES - D2 - P36
Sustainable protocol for direct reuse of platinum group metals from spent automotive catalysts

Zara Cherkezova-Zheleva[1], Anna Vasileva[1], Kaloyan Ivanov[1], Anastasia Maria Moschovi[2], Iakovos Yakoumis[2], Daniela Paneva[1]
[1]Institute of Catalysis, Bulgarian Academy of Sciences, Bulgaria; [2]MONOLITHOS Catalysts and Recycling Ltd, Greece

Sustainable management of platinum group metals (PGMs) requires strategies that retain value from spent catalysts while minimizing environmental burden. In contrast to conventional recycling schemes that focus on complete metal extraction and refining, direct reuse aims to preserve the PGM-containing solid as a functional catalytic entity. Here we propose a circular protocol in which spent catalyst substrates are converted into application-ready catalytic materials through mechanochemical treatment. The approach begins with comminution and classification to isolate PGM-enriched fractions, followed by conditioning that restructures the oxide support and redistributes PGM species without dissolving the matrix. Structural evolution is monitored by XRD and FTIR to track phase changes and functional groups, while XPS provides insight into PGM oxidation states and interactions with promoter oxides. SEM/EDS and TEM reveal morphology refinement, improved dispersion, and nanoscale PGM domains anchored to high-surface-area regions created during activation. From a process systems perspective, the proposed mechanochemical protocol reduces reliance on aggressive reagents and high-temperature operations, and it reduces energy requirements, processing complexity, and waste generation relative to extraction-centered routes. The proposed direct reuse pathway shifts recycling from metal recovery toward performance-driven upcycling, delivering catalytically active materials while maintaining traceability of composition and supporting reintegration into value chains. This strategy advances circular economy implementation for critical metals by prioritizing functionality, resource efficiency, and environmental impact reduction.

Acknowledgements: The authors gratefully acknowledge the support of project H2020-MSCA-RISE-2020 101007669: Chemistry of Platinum Group Metals, CHemPGM. Research equipment of the project № BG16RFPR002-1.014-0006 "National Centre of Excellence Mechatronics and Clean Technologies" was used for experimental work financially supported by European Regional Development Fund under "Research Innovation and Digitization for Smart Transformation" program 2021–2027.

EES - D2 - P37

Sustainable mechanochemical synthesis of molybdenum and Tungsten dichalcogenides for the hydrogen evolution reaction

Joseph D. Parkinson[1], A.R. Bonity J. Lutton Gething[2], Tomislav Friščić[2], Neil V. Rees[1]
[1]School of Chemical Engineering, University of Birmingham, UK; [2]School of Chemistry, University of Birmingham, UK

Transition Metal Dichalcogenides (TMDs) have seen extensive research into their activity towards the Hydrogen Evolution Reaction for the last 2 decades, with focus given to materials such as molybdenum and tungsten disulfide (MoS_2 and WS_2).Compared to platinum as the industry standard cathode, these materials boast lower costs, more sustainable production, and ease of modification, though lack activity in their bulk state due to an inactive basal plane. [1]

Despite this, microstructuring techniques can help remedy this inherent inactivity, for instance by preferentially exposing certain active sites, formation of heterostructures or doped species, or exfoliation to monolayers. [2,3] Mechanochemistry has been used to great effect exploring top-down modifications of the bulk, but synthesis and modification from the bottom-up remains unexplored, despite key advantages of bottom-up synthesis on catalytic activity, and recent precedent for the synthesis of similar materials despite molybdenum and tungsten varieties remaining elusive. [4,5,6] Such a method would demonstrate a versatile, sustainable, energy-efficient and scalable mechanochemical method to produce these essential catalysts; aligned with the key principles underlying Green and Sustainable Chemistry [7]

Hence, we present investigations into the bottom-up mechanochemical synthesis and modification of TMDs, using combined solvent-free and Liquid-Assisted approaches in an attempt to synthesise a range of chalcogenides. Synthetic conditions were varied to explore the optimal reaction pathway, along with characterisation of intermediates, for a more complete mechanistic understanding.

Acknowledgements: This work was supported by the Sustainable Hydrogen Centre for Doctoral Training, under EPSRC grant EP/S023909/1. The authors also thank the Nanoscale and Microscale Research Centre (nmRC) at the University of Nottingham for providing access to instrumentation, and Dr Hannah Constantin for technical assistance.

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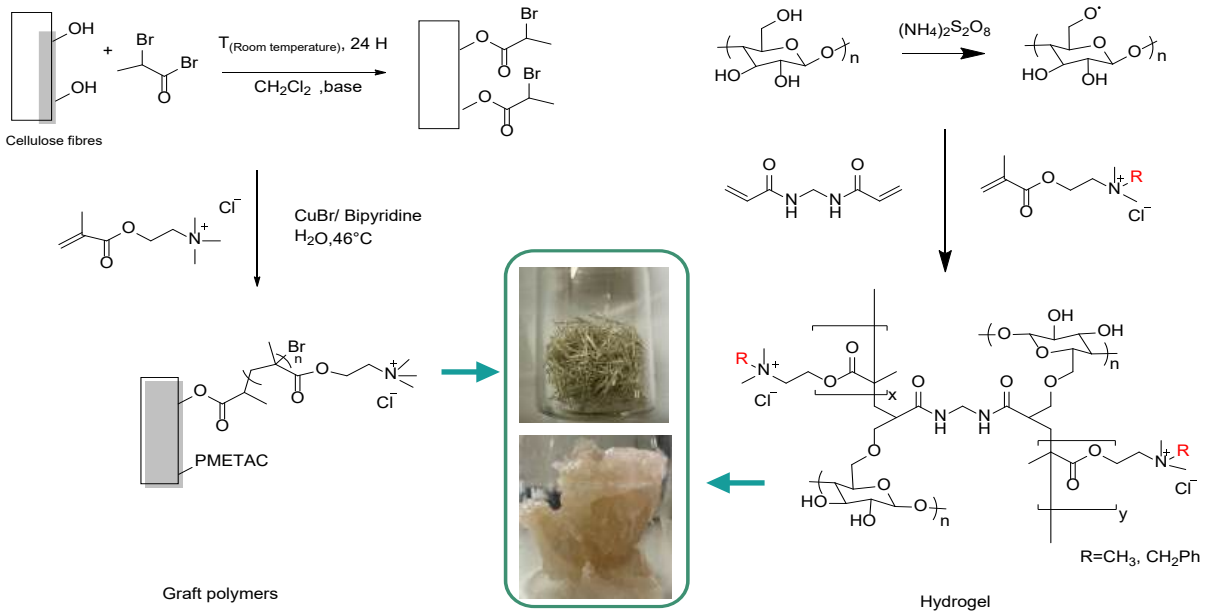
EES - D2 - P38

Preparation of cellulose-based adsorbents for eradication of pollutants in water

David Barker[1,2], Sumaira Basharet[1,2], Lisa I. Pilkington[1,3]

[1]School of Chemical Sciences, University of Auckland, New Zealand; [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand; [3]Te Pūnaha Matatini, New Zealand

Anionic pollutants such as (nitrates, phosphates, PFAS, NSAIDs, etc) pose a significant threat to both aquatic environments and public health. One means for removing these pollutants from water is by utilizing cationic adsorbents using ion-exchange. Commonly used anion exchange resins are typically derived from synthetic polystyrene-based polymers using toxic chemicals which are difficult to degrade and can be non-selective in their anion capturing efficiency. We will present how highly efficient, cellulose-based, water filtration systems were synthesized utilizing either atom transfer radical polymerization (ATRP) or free radical polymerization (FRP). Graft polymers were synthesized using cationic acrylamides grafting from a bromo-modified cellulosic backbone through ATRP giving highly porous fibre-based materials. Separately, cationic acrylamides were grafted onto cellulose via FRP initiated by ammonium persulfate using methylene bisacrylamide (MBA) as a cross linker which formed high absorbent cationic hydrogels. Comparative characterization of the ungrafted and grafted cellulose polymers was performed by Fourier-transform infrared spectroscopy (FTIR), Nuclear Magnetic Resonance (NMR) and Raman Spectroscopy. The results confirmed the successful synthesis of the novel cationic materials. Isothermal and kinetic studies were further studied to check the efficiencies of the prepared materials to bind nitrates, phosphates, PFAS and NSAID's. The results proved that cellulose grafted polymers serve as efficient green materials for anionic pollutant removal in wastewater.



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EES - D2 - P39

Design and characterization of new eco-friendly nitrobenzoxazine polymers with energetic potential

Thamer Gouasmia[1], Oussama Mehelli[1], Mehdi Derradji[1], Abdelmalek Habes[1]
[1]Ecole Militaire Polytechnique, Laboratoire de Génie des Procédés, UER Procédés Energétiques, Algiers, Algeria

The growing demand for sustainable high-performance materials has intensified interest in bio-derived thermosetting polymers with tunable energetic functionalities. Polybenzoxazines have emerged as promising candidates due to their excellent thermal stability, low moisture uptake, and versatile molecular design. In this study, we report the development of a new class of eco-friendly energetic polybenzoxazine precursors derived from eugenol, a naturally occurring bio-phenol, and functionalized with nitrogen-rich groups to impart enhanced energetic characteristics. Benzoxazine monomers were synthesized through a Mannich condensation reaction involving eugenol and nitroaniline as the nitrogen-containing co-reactant. Structural confirmation was achieved using 1H NMR spectroscopy, FTIR analysis, and elemental analysis, all of which verified the successful formation of the targeted benzoxazine frameworks. Thermal degradation behavior was evaluated by thermogravimetric analysis (TGA), revealing decomposition features consistent with materials intended for energetic applications. To complement the experimental investigation, Machine Learning (ML) techniques were applied to validate critical measured properties, including density (d) and decomposition temperature (Td), and to predict key energetic performance indicators such as detonation velocity (Dv) and detonation pressure (P). The ML models exhibited strong predictive accuracy, reinforcing the reliability of the experimental data and providing valuable insights into the energetic potential of the synthesized materials. Overall, this work highlights the effective integration of bio-based feedstocks with data-driven approaches to advance the design of next-generation sustainable energetic polybenzoxazines.

EES - D2 - P40

Experimental investigation of antibacterial properties and mechanical performance enhancement of sintered seashell–reinforced poly(lactic acid) and poly(butylene succinate) biocomposites planned for 3D printing

Mohammed Seddik Razali[1], Kamel Khimeche[1], Hichem Dahah[1], Nourddine Ramdani[1]
[1]Military Polytechnic school, Chahid abderahmen Taleb, Algeria

To date, the development of biodegradable, so-called green, composites combining natural or bio-based fibers with environmentally friendly resins has emerged as an effective approach to enhance the mechanical properties of biocomposites [1]. Seashells have been widely investigated as reinforcement materials due to their low cost, low density, thermal stability, biodegradability, recyclability, and sustainability [2]. Seashell-derived bioceramics from marine resources have shown strong potential for reinforcing biopolymers in biomedical applications [3]. Their biocompatibility and biodegradability make them suitable for medical implants, tissue engineering, and drug delivery systems [4, 5], while also contributing to environmental sustainability [6].

On the other hand, the rapid progress of additive manufacturing technologies, especially 3D printing, has led to significant advances in biomedical applications [7]. Although fused filament fabrication (FFF) facilitates the fabrication and prototyping of medical devices, controlling and minimizing the risk of contamination remains a major concern. As a result, new antibacterial materials, including polymer composites incorporating silver nanoparticles, have recently been introduced to the market [8].

In this study, a newly sintered seashell filler (SSh) was prepared from bio-based seashells collected along the Mediterranean coast using a suitable heat treatment process. Structural analysis confirmed that the SSh filler was mainly composed of calcium oxide, while BET analysis showed a significant increase in specific surface area compared to the raw powder. Morphological observations using SEM indicated a wing-like structure, which is favorable for mechanical reinforcement.

Subsequently, a series of PLA- and PBS-based biocomposites containing different SSh contents (5, 10, 20, and 30 wt.%) were prepared using a twin-screw extruder to produce filaments for (FFF) fabrication. The antibacterial activity of this biocomposites was evaluated against Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*) and Gram-positive bacteria (*Staphylococcus aureus*). The PLA-based biocomposite containing 20 wt.% SSh exhibited inhibition zones of 8 mm and 6 mm against *E. coli* and *P. aeruginosa*, respectively, while no antibacterial activity was observed against *S. aureus*. Moreover, the mechanical properties and microhardness of the biocomposites increased with increasing filler content due to the high rigidity of the SSh biofiller.

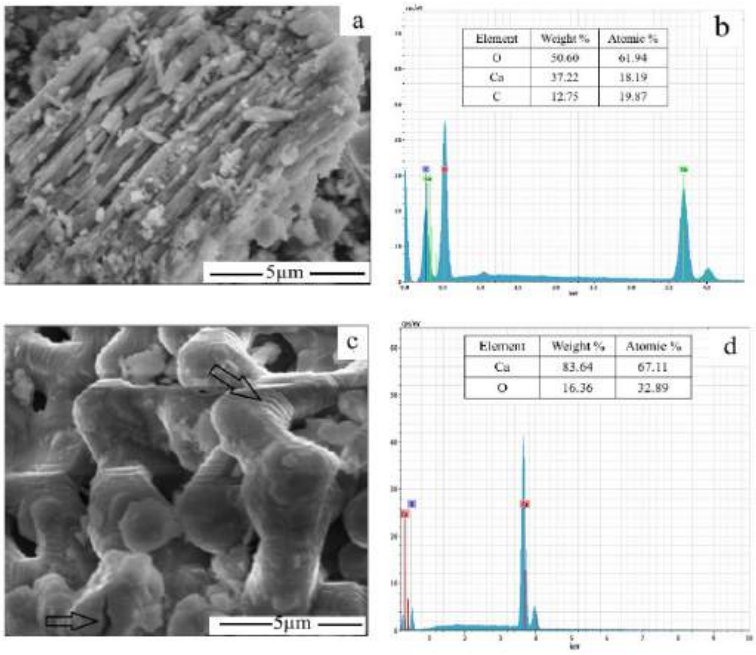

Fig. 1. SEM-EDX micrographs of: **(a, b)** Seashell (crushed raw powder), **(c, d)** Sintered seashell powder.

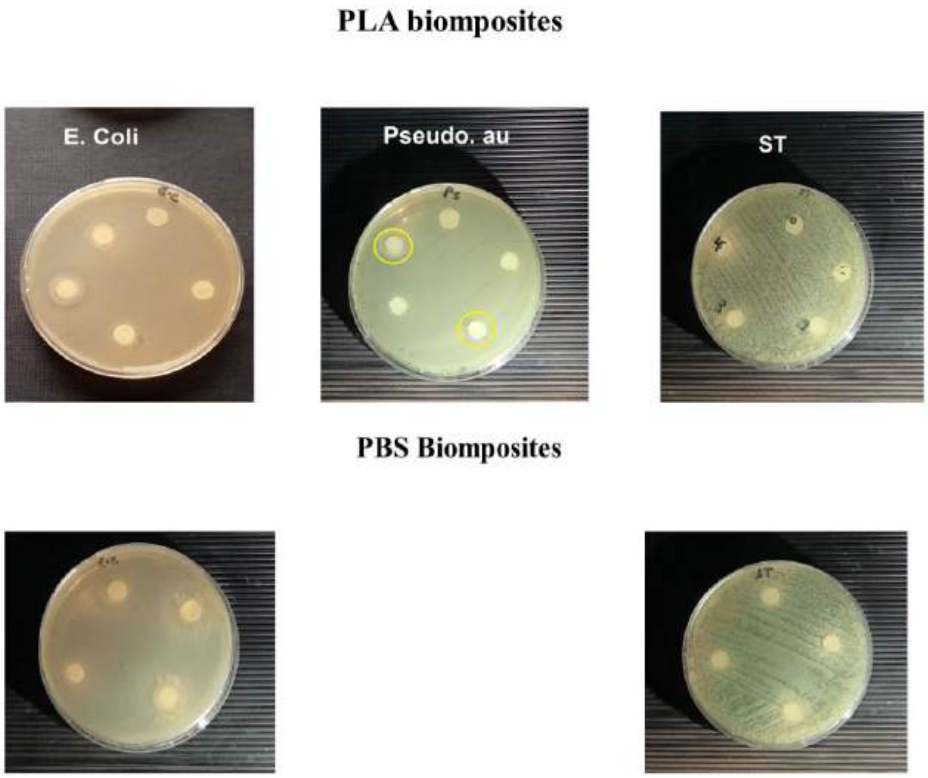

Fig. 2. Antibacterial assay of PLA and PBS based biocomposites: zone of inhibition against (1) Escherichia coli (E.coli), (2) Pseudomonas aeruginosa (Ps. au) and (3) Staphylococcus aureus (ST).

Table I- Tensile properties parameters of elaborates poly(lactic acid) (PLA)/SSh and PBS/SSh biocomposite filaments.

sample	Tensile strength (MPa)	Elongation at break (%)	Young's modulus (MPa)
PLA	29.81 (±1.8)	2.19	183.78 (±4.69)
PLA/5 SSh	43.66 (±4.02)	2.32	232.70 (±29.96)
PLA/10 SSh	49.06 (±8.87)	2.36	241.86 (±63.02)
PLA/20 SSh	25.78 (±6.52)	1.87	180.92 (±8.99)
PLA/30 SSh	17.05 (±4.87)	1.34	158.86 (±9.21)
PBS	3.53 (± 0.77)	1.62	217.9 (± 14.5)
PBS/5 SSh	4.94 (± 0.19)	1.52	325 (± 12.5)
PBS/10 SSh	5.06 (± 0.22)	0.92	550 (± 23.9)
PBS/20 SSh	6.77 (± 0.86)	0.79	856.9 (± 48.8)
PBS/30 SSh	4.12 (± 0.74)	0.48	858.3 (± 54.1)

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EES - D2 - P41

Optimization of the polycyclic aromatic hydrocarbons (PAHs) removal process in wastewater using MXene-supported activated carbon (MX-AC) material

Hifsa Khurshid[1], Muhammad Raza Ul Mustafa[2], Saviour A. Umoren[1], Rami K. Suleiman[1]
[1]Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia; [2]Centre for Urban Resource Sustainability, Institute of Self-Sustainable Building, Dept. of Civil & Environmental Engineering, Universiti Teknologi Petronas, Malaysia

The presence of polycyclic aromatic hydrocarbons (PAHs) in industrial wastewater poses significant environmental and health risks, necessitating efficient and scalable treatment strategies [1]. In this study, a novel composite adsorbent based on MXene ($Ti_3C_2T_x$)–supported activated carbon (MX-AC) was synthesized and optimized for the removal of representative PAHs from aqueous systems [2,3]. The composite was prepared via aqueous dispersion of MXene nanosheets with oil-palm-leaf–derived activated carbon. Adsorption performance was evaluated in batch testing using naphthalene (NAP), fluorene (FLU), and phenanthrene (PHE) as model contaminants [4]. Process optimization was conducted using Response Surface Methodology coupled with a Central Composite Design to assess the effects of solution pH (3–9), adsorbent dosage (100–3000 mg L^{-1}), and contact time (5–90 min) [5]. ANOVA confirmed a statistically significant quadratic model for all three analytes (model F–values 22.26–57.60, $p \leq 0.0001$), with excellent agreement between predicted and adjusted coefficients of determination (e.g., NAP: $R^2_{adj} = 0.9254$, $R^2_{pred} = 0.7448$; FLU: $R^2_{adj} = 0.9542$, $R^2_{pred} = 0.8376$; PHE: $R^2_{adj} = 0.9706$, $R^2_{pred} = 0.8993$). Response surface analysis revealed strong interactions among variables, particularly the beneficial combined effects of low pH and higher dosage up to an intermediate contact time (~45–70 min), beyond which efficiency diminished as shown in Figure 1. Numerical optimization identified optimal operating conditions at pH 3, an MX-AC dosage of approximately 1493 mg L^{-1}, and a contact time of about 67 min, yielding predicted removals of 94.2% for NAP, 99.0% for FLU, and 98.2% for PHE. Experimental validation closely matched these predictions. When applied to real produced water from the oil and gas industry under optimized conditions, the composite achieved approximately 90% removal of all target PAHs, demonstrating robustness in complex matrices, as shown in Table 1. Overall, the MX-AC composite exhibits high efficiency and practical potential for PAH remediation.

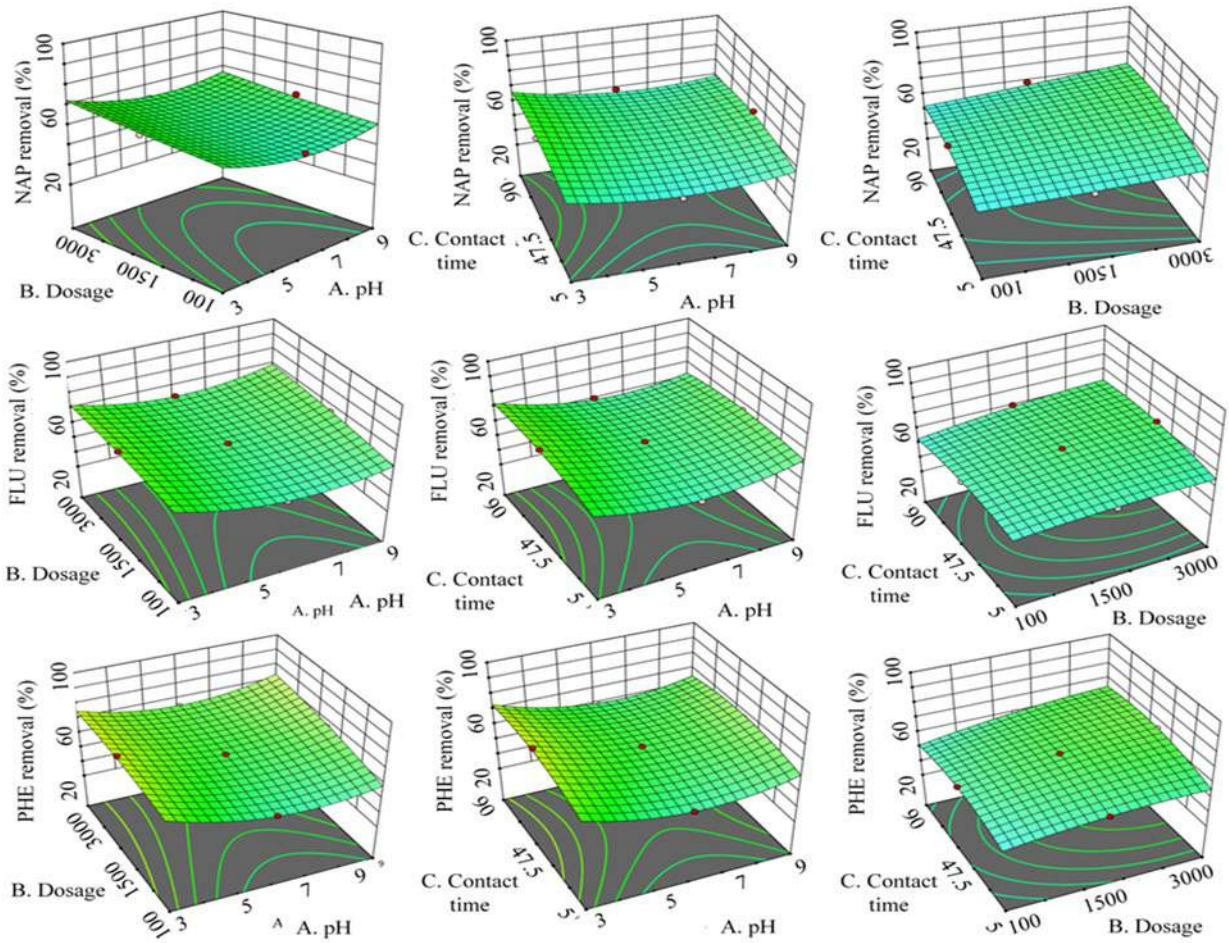

Fig. 3. Impact of pH, MX-AC dosage and contact time on adsorptive removal percentage of NAP, FLU and PHE

Table 1. Optimized results of adsorption

Material	Pollutants removed	A	B	C	RSM Predicted removal (%)	Removal in synthetic aqueous solution (%)	Removal in wastewater from industry (%)
MX-AC	NAP	3	1493	67	94.2	95	90.89
	FLU				99	99.3	90.2
	PHE				98.23	96.3	90.2

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EES - D2 - P42

Synthesis and characterization of sol–gel–derived Co/SiO_2 nanocomposites for electrochromic applications

Daouia Brahmi-Ingrachen[1], Sylia Azoug[1]

[1]University of Bejaia, Faculty of Exact Sciences, Laboratory of Materials Technology and Process Engineering (LTMGP), Algeria

Electrochromic (EC) materials have been the focus of scientific and technological research for over three decades due to their potential in energy-saving smart windows and large-area displays. EC devices operate via reversible coloration and bleaching cycles under low alternating voltages, making them highly attractive for industrial and commercial applications.

In this study, cobalt nanoparticles were synthesized through a sol–gel approach. Cobalt(II) nitrate hexahydrate was evaluated as a precursor, while a stable silica sol was prepared from kaolin-derived siliceous by-products. The cobalt precursor was incorporated into the silica sol to form a Co/silica solution, which was then deposited onto glass substrates using the dip-coating technique to obtain thin films. Initially amorphous, the films developed a crystalline structure following heat treatment at 500 °C. Electrochemical tests revealed a positive electrochromic response of the Co–SiO_2 films in 1 M KOH, confirming their suitability for EC applications. Structural and chemical characterizations using X-ray diffraction (XRD), UV–Vis spectroscopy, and cyclic voltammetry (CV) demonstrated well-dispersed cobalt nanoparticles within the silica matrix and excellent electrochemical stability.

This work presents a simple and efficient strategy for producing cobalt–silica-based EC films from industrial by-products, offering a sustainable and cost-effective route for next-generation electrochromic devices. The approach combines material innovation with environmental considerations, highlighting its potential for scalable and practical applications.

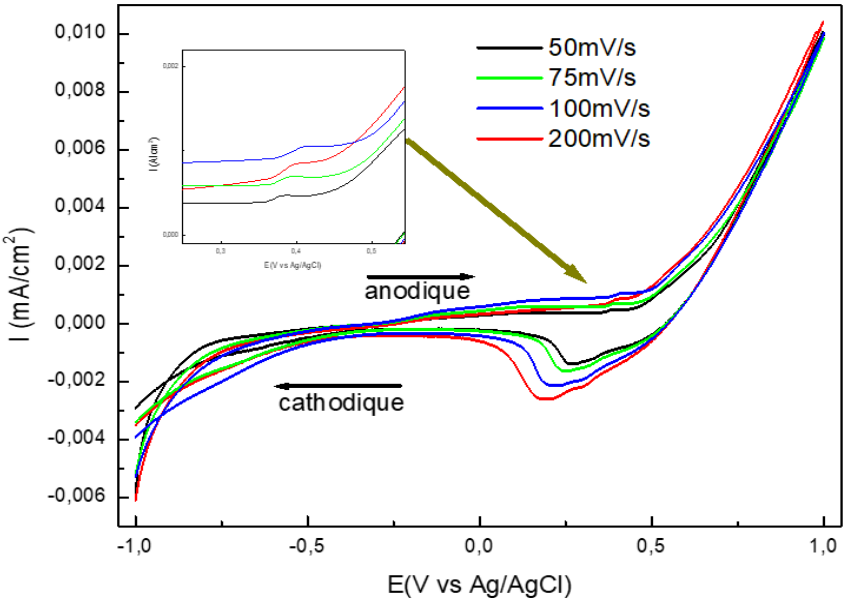

Fig. 1. The cyclic voltammograms of the films calcined at 500 °C for 60 minutes at different scan rates.

EES - D2 - P43

Development of a superhydrophobic nonwoven polyester membrane for efficient and scalable oil-water separation: Eco-friendly fabrication and performance evaluation

Abdul Saeed[1], Zulfiqar Ahmed Rehan[2]
[1]Institute of Solid-State Physics, Hefei Institutes of Physical Science, Chinese Academy of Sciences, China; [2]Dept. of chemistry, college of Science, Sultan Qaboos University Muscat, Oman

The growing environmental concerns related to industrial oily wastewater and offshore oil spills highlight the urgent need for efficient, durable, and cost-effective oil-water separation technologies. This study presents the fabrication of a novel superhydrophobic nonwoven polyester (NWP) membrane using eco-friendly sol-gel and phase inversion methods. The membrane was synthesized by integrating polyvinylidene fluoride (PVDF) and polyvinylpyrrolidone (PVP) with hydrolyzed tetraethyl orthosilicate (TEOS) and vinyltris(2-methoxyethoxy)silane (VTMEOS), resulting in a robust and highly porous composite structure. The membrane exhibited exceptional hydrophobicity, with a water contact angle exceeding 150°, and demonstrated excellent mechanical and chemical stability across a pH range of 1–13. In a custom-built low-pressure filtration device (0.02 MPa), the hydrophobic membrane achieved an ultra-high flux rate of 19,400 Lm−2h−1 and a separation efficiency of 99.9% over 70 filtration cycles. The membrane's porosity (87.17%) and finely tuned pore size distribution (0.4–1.8 μm) significantly enhanced its separation performance. Density Functional Theory (DFT) calculations confirmed the chemical interactions responsible for the surface modification and hydrophobic behavior. This study introduces a scalable, energy-efficient membrane system, offering a promising solution for next-generation oil-water separation in environmental remediation.

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EES - D2 - P44

Fabrication of 2D/1D S-scheme Pg-C3N4/Ag3VO4 nanocomposite with high interfacial charge separation for highly selective photoconversion of CO2 into Fuels

Abdullah Bafaqeer[1*]

[1]Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia

Well-designed template free synthesis of 2D protonated graphitic carbon nitride nanosheets (Pg-C3N4) coupled with 1D Silver vanadium oxide nanorods (Ag3VO4) to construct 2D/1D interface heterostructures with strong electrostatic interactions between positively charged 2D Pg-C3N4 nanosheets and negatively charged 1D Ag3VO4 nanorods has been investigated. The coupling of Pg-C3N4 and Ag3VO4 with good characteristics resulted in 2D/1D interface heterojunction with S-scheme mechanism for charge carrier transfer by maintaining and effectively using useful charge carriers. The 2D/1D Pg-C3N4/Ag3VO4 exhibited remarkable photocatalytic performance for CO2 conversion with H2O resulting in maximum CH4 production of 352.3 µmole/g-cat. Compared to Pg-C3N4 samples, the optimized 2D/1D Pg-C3N4/Ag3VO4 nanocomposite exhibited 2.9-fold higher efficiency in CH4 production, highlighting the advantages of their structure. Similarly, the Quantum yield of 0.23% for CH4 generation was obtained over 2D/1D Pg-C3N4/Ag3VO4, which was 2.9 and 1.4 times higher than Pg-C3N4 and Ag3VO4 samples, respectively. The improvement in photocatalytic performance primarily stems from the effective interaction between Pg-C3N4 and ternary Ag3VO4, leading to enhanced transfer and separation of photoinduced charge carriers through the creation of an S-scheme heterojunction. Additionally, the optimum Pg-C3N4/Ag3VO4 nanocomposite demonstrated high photostability after repeated experimental runs with no discernible variations. The utilized photocatalyst displayed no change in morphology, thus proving further good stability of the Pg-C3N4/Ag3VO4 photocatalyst. The findings of this study would be useful in designing template-free heterojunctions for photocatalytic CO2 conversion and other solar energy applications.

EES - D2 - P46

Electrochemical CO_2 conversion to formic acid using bismuth nanoparticle electrocatalysts

Muhammad Usman[1], Munzir Sulaiman[1], Niamat Ullah[1], Neelam Zaman[1], Muhammad Ajmal[1]
[1]Interdisciplinary Research Center for Hydrogen and Carbon Management (IRC-HTCM), King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia

Metal-organic frameworks (MOFs) based electrocatalysts for CO2 reduction offer unique possibilities for developing advanced materials for this reaction due to their ordered nanoporosity and pore environments, tunable characteristics, and high affinity for CO2. Still, they were not investigated sufficiently. In this study, we developed a Bismuth nanoparticles embedded in MOFs via a facile synthesis method for the electrochemical CO_2 reduction reaction (eCO_2RR). Comprehensive spectroscopic and electrochemical characterization confirmed the successful synthesis of bismuth in MOFmatrix. The electrocatalytic performance was assessed in multiple reactor typologies such as H-cell, flow cell, and membrane electrode assembly (MEA) setups. Remarkable differences in the performances in the three cell configurations are evidenced. Notably, the MEA configuration exhibited a marked enhancement in formate selectivity, achieving a Faradic efficiency (FE) of up to 90 % at a high current density of −150 mA cm–². This work underscores the potential of bismuth and MOFs composites in advancing eCO_2RR while remarking on the crucial importance of the appropriate type of electrocatalytic experiments in assessing the material performance.

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EES - D2 - P47

Polyaniline/nanocellulose/ MXene hybrid nanocomposites as greener and sustainable electrocatalysts for efficient oxygen evolution reaction

Tahir Rasheed[1]
Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia

Herein, three different polyaniline, nanocellulose and molybdenum carbide (Mo_2C_3) (PANI-Mo-NC-1, 2 and 3) based electrode materials were prepared by varying the mass ratios of the components through mechanical mixing followed by freeze drying to catalyze the oxygen evolution reaction (OER). The prepared electrode materials were characterized by using different techniques i.e. SEM, TEM, XRD and FTIR etc. the electrochemical measurements were carried out in 1M KOH solution. The cyclic voltammetry (CV) of as prepared electrodes with different compositions were recorded at scan rates ranging from 5 to 100 mV s^{-1}. All samples exhibit well-defined anodic and cathodic redox peaks in the potential window of ~0.9-1.2 V vs. RHE, which are characteristic of the reversible redox transitions. The overpotentials required to reach a current density of 10 mA cm^{-2} are calculated to be 112 mV, 92 mV, and 132 mV for (PANI-Mo-NC-1,2 and 3) respectively. Further the calculated Tafel slopes are in the order of 83.0 mV dec^{-1}, 72.0 mV dec^{-1}, and 101.0 mV dec^{-1} respectively. The lowest overpotential and Tafel slope of PANI-Mo-NC-2 reflects the most favorable reaction energetics and fastest OER kinetics. This suggests that the rate-determining step for OER is facilitated by optimal Mo_2C_3 loading, likely through improved adsorption/desorption of oxygenated intermediates. The results indicate that the electrode PANI-Mo-NC-2 is identified as most promising catalyst for potential OER due to its performance as well as its chemical and electrochemical robustness.

Keywords: Greener and sustainable; conductive polymer; MXene; water splitting; oxygen evolution; electrocatalyst.

EES - D2 - P48
Conversion of CO_2 to value-added products over a Ca and Cu modified UiO-66 catalyst

Tani Monene[1], Mduduzi Cele[1]
[1]North-West University, South Africa

Carbon dioxide (CO_2) is increasing continuously in the atmosphere due to the burning of fossil fuels, contributing to global warming and other natural disasters. CO_2 conversion is one of the most promising methods for reducing CO_2 in the atmosphere to produce sustainable chemicals, fuel, and renewable energy. Products like methanol and formic acid are of high value and are ideally produced through the hydrogenation of CO_2. Metal-organic frameworks (MOFs) are attractive catalysts in CO_2 utilisation due to their high surface area and tailorability of metal nodes and organic ligands. This study focuses on the conversion of CO_2 to green methanol using modified Zr-UiO-66 catalysts at temperatures below 200 °C. The MOFs are synthesised using a co-precipitation method that incorporates copper and calcium to promote CO_2 conversion and high methanol selectivity. The synthesised Zr-UiO-66, Cu/Zr-UiO-66, Ca/Zr-UiO-66 and CaCu/Zr-UiO-66, catalysts were characterised using FTIR, XRD, TGA, BET, SEM and TEM. The XRD and FTIR confirmed the successful synthesis of all the UiO-66 catalysts by providing XRD patterns and functional groups corresponding to the standard UiO-66 MOF. TGA analysed the thermal stability of synthesised UiO-66 catalysts, and they were all thermally stable up to 482 °C. The BET results indicate a surface area ranging from 600 to 800 m^2/g. At the same time, EDS confirms the presence of Cu, Ca and Zr in the catalysts. Methanol and formic acid products were observed from the hydrogenation of CO_2 at 100 °C, with Ca-modified catalysts being the most active.

EES - D2 – O07

Liquid–solid phase separation-assisted direct CO_2 capture from air with a new system

Xiaopan Xue[1], Xuanbing Li[1], Soichi Kikkawa[1], Hideyuki Kawasok[1], Seiji Yamazoe[1]
[1]Graduate School of Science, Tokyo Metropolitan University, Japan

Direct air capture (DAC) of CO_2 has attracted significant attention as an effective strategy to reduce atmospheric CO_2 levels.[1] In our previous studies, a liquid–solid phase separation system based on isophorone diamine (IPDA) and carbamic acid exhibited efficient CO_2 absorption at 400 ppm,[2] and aqueous solution of IPDA was shown to react with CO_2 at a 1:1 molar ratio when CO_2-containing gas was introduced by bubbling.[3] However, conventional bubbling processes suffer from pressure loss and sorbent vaporization, while solvent-based systems require excess energy for heating during CO_2 desorption.

To overcome these limitations, we developed a new system CO_2 absorption reactor that minimizes sorbent usage while maintaining high gas–liquid contact efficiency. Using this reactor, more than 90% of CO_2 (400 ppm) was continuously removed for 1153 min with 1.0 mmol of IPDA under H_2O vapor, achieving a total CO_2 uptake of 1.12 mmol. FT-IR analysis confirmed the coexistence of carbamic acid and bicarbonate species. In comparison, a conventional bubbling-type reactor using 1.0 mmol of IPDA and 1 mL of H_2O captured 1.00 mmol of CO_2 under identical conditions, indicating that the new system enables efficient CO_2 capture with reduced solvent usage. By contrast, neat IPDA under dry conditions showed lower performance, capturing only 0.64 mmol of CO_2, highlighting the critical role of H_2O vapor in reducing viscosity and enhancing gas–liquid contact. CO_2 desorption was achieved by treating the CO_2-loaded sorbent with methanol at 60 °C, following a reported procedure.[4] Confirming the effectiveness of the new system reactor for efficient and sustainable DAC.

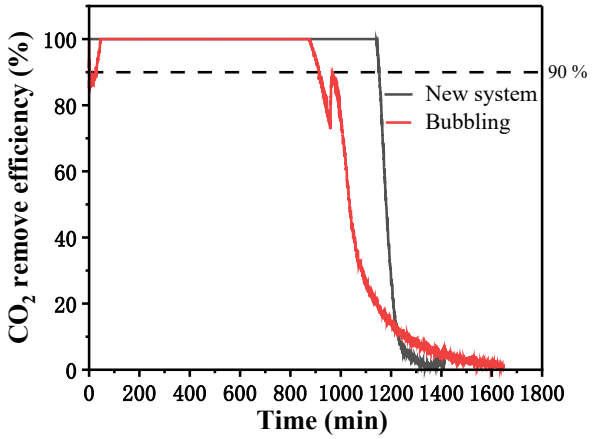

Fig. 1. CO_2 removal efficiency of IPDA evaluated using a bubbling-type reactor and a new system reactor.
Absorption condition: IPDA, 1.0 mmol, 400 ppm CO_2, 50 mL/min. Temperature, ambient.

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EES - D3 - P01
Greener synthetic approaches to the synthesis of quinoxaline derivatives

Daniela Andrei[1], Griselda Jaupi[1], Brian Alvarado[1], Kaya Jakowczuk[1]
[1]Dominican University, River Forest, IL, USA

Quinoxaline derivatives are an important class of nitrogen-containing heterocycles with applications in medicinal chemistry, materials science, and fluorescence-based sensing. However, many reported synthetic routes rely on hazardous solvents, excess reagents, and energy-intensive conditions, limiting their sustainability and suitability for instructional laboratories. This work explores greener synthetic strategies for the preparation of quinoxaline derivatives while engaging undergraduate students in environmentally responsible research.

A series of quinoxaline derivatives was synthesized via the condensation of substituted *o*-phenylenediamines with 1,2-dicarbonyl compounds using both traditional and green chemistry–inspired approaches. Conventional methods employing organic solvents and prolonged heating were compared with modified protocols that incorporate ethanol as a greener solvent, reduced reagent loading, and milder reaction conditions. In select cases, less hazardous reagents were evaluated as substitutes for commonly used alternatives. Reaction progress was monitored by thin-layer chromatography, and products were characterized using infrared spectroscopy, nuclear magnetic resonance spectroscopy, and UV–visible spectroscopy.

Comparative analysis demonstrated that the greener methods provided comparable or improved yields while significantly reducing solvent toxicity, waste generation, and overall environmental impact. These results illustrate that sustainable synthetic practices can be successfully implemented without compromising reaction efficiency or educational value. Importantly, this work highlights the feasibility of integrating green chemistry principles—such as safer solvents, waste minimization, and improved atom economy—into undergraduate research and teaching laboratories.

Beyond the synthetic outcomes, this project serves as a model for incorporating green chemistry into undergraduate education through hands-on research. The approach reinforces core concepts in organic synthesis while fostering student awareness of sustainable laboratory practices. This study supports the broader adoption of green chemistry methodologies in academic settings and demonstrates their value in both research and pedagogy.

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EES - D3 - P02
CO_2 upcycling to liquefied petroleum gas and jet fuel via an oxide–zeolite catalyst strategy

Kyungsu Na[1]
[1]*Chonnam National University, Dept. of Chemistry, Gwangju, Republic of Korea*

Sustainable aviation fuels (SAF) synthesized via Power-to-Liquids (PtL) processes utilizing CO_2 and green hydrogen represent a critical pathway for decarbonizing the aviation industry. However, synthesizing jet fuels through CO_2 hydrogenation presents challenges in overcoming the Anderson–Schulz–Flory distribution and optimizing the olefin-to-paraffin ratio to meet strict fuel specifications. This study proposes an oxide–zeolite (OXZEO) strategy to produce jet-range paraffins using a bifunctional catalytic system comprising an Fe-K supported copper aluminum spinel (FKC) oxide catalyst and a proton-form MFI zeolite. To enhance the diffusion of bulky $C_{8\text{-}16}$ hydrocarbons, a mesoporous nanosheet-type zeolite (NS) was introduced and loaded with Pt metal to facilitate olefin hydrogenation. In-situ DRIFTS analysis revealed that the NS catalyst with 1 wt% Pt exhibits superior hydrogen dissociation capabilities due to a high surface Pt^0 ratio. This functionality promotes formate formation in the FKC, shifting the thermodynamic equilibrium toward CO_2 consumption while simultaneously enhancing the hydrogenation of olefins. Consequently, this catalytic design achieved the highest paraffin ratio within the $C_{8\text{-}16}$ composition, demonstrating a practical approach for effective CO_2 upcycling into high-quality aviation fuel.

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2024-00466475 and RS-2024-00349276).

EES - D3 - P03
Understanding the effects of cryomilling for some common thermoplastics

Niloofar Kamyar[1], Mahnam Ebadi[1], Bilge Baytekin[1]
[1]Bilkent University, Turkey

It has been known since the times of Staudinger[1] that mechanical force can break polymer chains by cleaving chemical bonds. This simple phenomenon can be used for beneficial purposes, such as in polymer recycling[2], mechanochemical copolymerization reactions, or other chemical reactions initiated by the generated mechanoradicals[3] (or to mitigate adverse effects like static charging caused by these radicals[4]). However, the vigorous, seemingly uncontrolled milling process does not provide the necessary 'fine' processing for these purposes. Yet, with global annual thermoplastic production of 445 million tons (290 billion dollars in value) and the growing need to reuse polymer materials, ball milling can be harnessed to deliver useful products.
This study involves cryomilling of some common polymers, polyethylene, polypropylene, polystyrene, poly(vinylchloride), and polyethylene terephthalate, which are the main players in the plastics market today. Cryomilling[5] must be used to avoid mastication of plastics and to increase bond-breaking efficiency. As the process itself also consumes energy and liquid nitrogen, polymers were milled for short durations (up to 10 minutes) to yield the desired structural and chemical changes in the selected polymers. Each milling parameter, such as jar material, milling frequency, and ball count, was evaluated for its effect on the overall bond-breaking process. In these analyses, the molecular weights of the polymers were monitored by gel permeation chromatography (GPC), oxidation of the milled material was tracked by X-ray photoelectron spectroscopy (XPS), and changes in crystallinity were determined by X-ray diffraction (XRD), along with other complementary characterization techniques. Quantitative analyses of the mechanoradicals formed during the milling were carried out by 2,2-diphenyl-1-picrylhydrazyl (DPPH) tests.[6] The results show that, depending on the chemical structure and crystallinity of the milled material, the milling outcome can be drastically different. Depending on the polymer structure, bond breakage can be heterolytic or homolytic, thereby diversifying the chemical species obtained.[7]

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EES - D3 - P04

Unraveling the electrocatalytic performances and structural stability of Ag nanowire gas diffusion electrodes for CO_2 reduction

Ola Bajouk[1,2,3], Bhavani Ravi[1], Elhassan Amaterz[4], Isabelle Rougeaux[4], Bertrand Reuillard[2], Elise Lorenceau[3], Pascale Chenevier[1]

[1]Univ. Grenoble Alpes, CEA, CNRS, GrenobleINP, IRIG, SYMMES, Grenoble, France; [2]Univ. Grenoble Alpes, CEA, CNRS, IRIG, LCBM, Grenoble, France; [3]Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France; [4]Univ Grenoble Alpes, CEA, Liten, DTNM, Grenoble, France.

The electrochemical reduction of CO_2 (eCO_2RR) offers a sustainable route for converting CO_2 into more value-added products, with carbon monoxide being a key component of syngas and in other industrial processes.[1] Among the range of catalysts explored for the selective electrochemical reduction of CO_2 to CO, silver has received considerable attention. In particular, silver nanowires (AgNWs) are distinguished by their high electrical conductivity, tunable morphology, and large electrochemically active surface area.[2] In this work, AgNW gas diffusion electrodes (GDEs) synthesized from a modified polyol method, were evaluated for eCO_2RR under different reaction environments and cell configurations. Reasonable faradaic efficiency for CO, exceeding 90%, could be obtained at –1.7 and –1.8V vs Ag/AgCl in 3-electrode flow cell setup and at cell voltage between 2.8 and 3V in zero gap electrolyser setup with a catalyst load of 0.2 - 0.3 mg/cm^2. Long term electrolysis tests showed stable operation for approximately 8 hours, followed by a gradual decline in CO selectivity, primarily attributed to salt precipitation and pore blockage within the GDE and the flow channels. Variation of CO_2 flow regimes demonstrated that reduced gas flow enhanced overall CO_2 conversion efficiency, up to 34% at 3.5V, compared to 12% at higher flow rates. Post-electrolysis characterization of the AgNWs surface revealed partial removal of the polyvinylpyrrolidone (PVP) capping layer and important morphological alterations in the nanowire network, though the overall catalytic activity remained largely preserved.

Keywords: CO_2 reduction reaction, Ag nanowire, Gas diffusion electrodes, Conversion efficiency, Morphological instability

EES - D3 - P05
Pilot-scale online monitoring of CESAR1 solvent condition in a cement CO_2 capture plant

Ward Peeters[1], Randi Neerup[1], Sergey Makarychev-Mikhailov[2], Maria Dimitriadi[1], István Györbíró[1], Mads F. Hennings[1], Philip L. Fosbøl[1]
[1]Technical University of Denmark (DTU); Dept. of Chemical Engineering, Center for Energy Resources Engineering (CERE), Denmark; [2]SLB Cambridge Research, UK

Chemical CO_2 capture using amine-based solvents is a cornerstone technology for achieving deep decarbonization in hard-to-abate industrial sectors such as cement production[1]. Despite advances in solvent energy efficiency and degradation resistance, solvent degradation remains a major challenge for reliable long-term operation of industrial-scale capture plants, leading to solvent loss, corrosion, and increased operating costs. Now solvent condition is mainly assessed through periodic sampling and labour-intensive offline analyses, resulting in delayed feedback and limited ability to implement proactive mitigation strategies.
This work presents the development and pilot-scale deployment of an online monitoring approach based on liquid-phase Fourier Transform Infrared (FTIR) spectroscopy for continuous assessment of the CESAR1 solvent system. The study is conducted at a continuously operated CO_2 capture pilot plant at a cement production facility in Aalborg, Denmark. The installation has a capture capacity of approximately 1 ton CO_2 per day[2]. CESAR1, a blend of 2-amino-2-methyl-1-propanol (AMP) and piperazine (PZ), is monitored online, including AMP and PZ concentrations, CO_2 loading, and solvent degradation behaviour. An in situ FTIR probe installed directly in the solvent loop enables high-frequency spectral acquisition without sampling or process interruption (**Figure 1**).

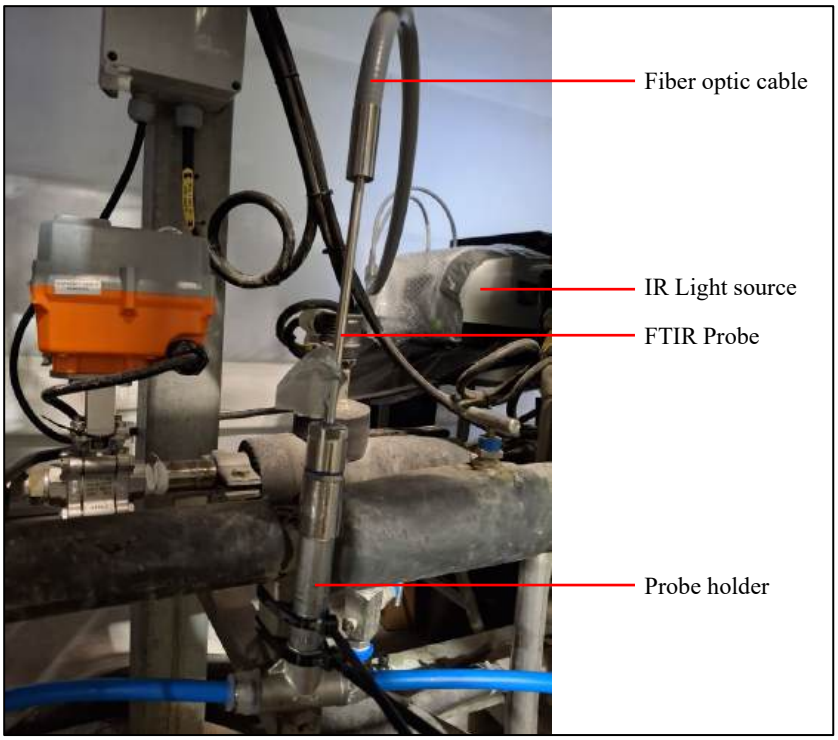

Fig. 1. In-situ FTIR probe connected to IR light source by a fibre optic cable

Quantitative interpretation of the FTIR data is done through offline reference analyses using ion chromatography, which are used to correlate characteristic spectral features with solvent composition, CO_2 loading, and degradation indicators. Machine learning models were trained and optimized using pilot plant data complemented by laboratory-prepared samples. Representative model validations for AMP and a characteristic degradation marker are shown in **Figure 2**, demonstrating agreement between predicted and measured concentrations across the observed operating range.

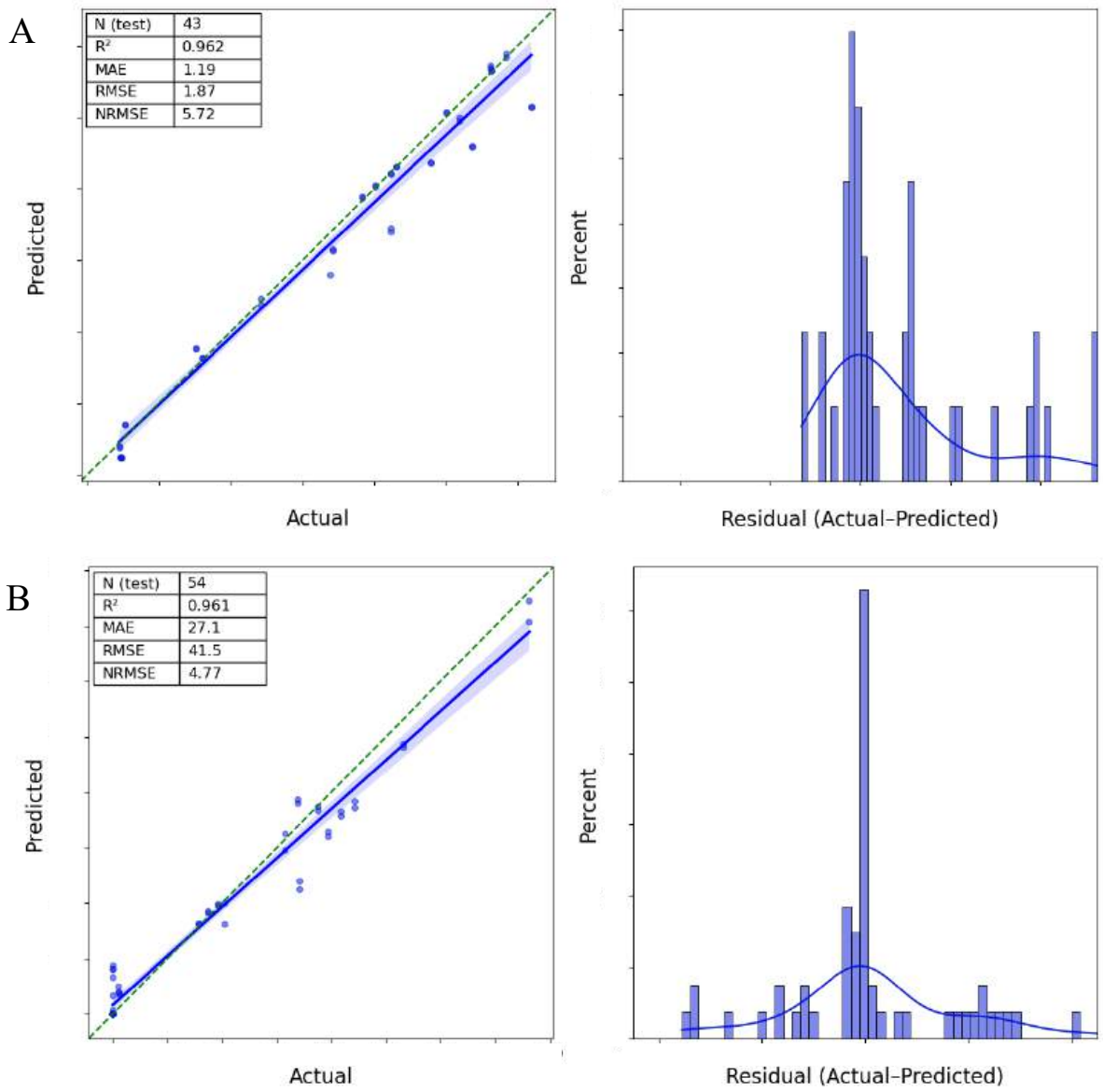

Fig. 2. A) Validation of a PLS model of AMP B) Validation of a PLS model of a specific solvent degradation marker

The continuous nature of the monitoring overcomes the limitations of periodic sampling, making it possible to detect degradation trends and support proactive operational strategies such as optimized solvent reclaiming and real-time evaluation of degradation inhibitors. Overall, the results demonstrate that in situ FTIR spectroscopy is a promising tool for online solvent monitoring in CO_2 capture applications.

Acknowledgements: The authors would like to acknowledge funding provided via the European Commission's Horizon Europe research and innovation program under the Marie Skłodowska-Curie Grant Agreement ID: 101118369, Material Science Innovation for Accelerated, Sustainable and Safe Implementation of Carbon Capture and Storage (MISSION-CCS), the financial support from the CASPER project, funded by INNO-CCUS (pool 2 no. 1-P8), the support of Art Photonics, and the support of the Technical University of Denmark (DTU).

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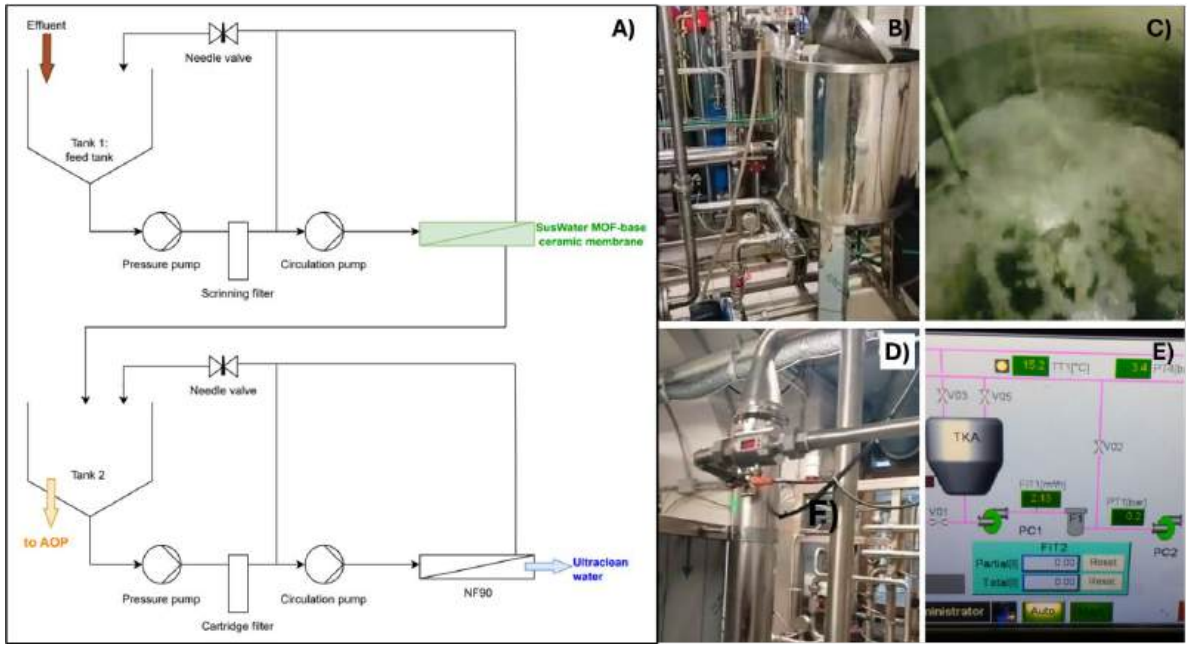
EES - D3 - P06

Sustainable integrated approach for CECs removal in aquaculture: Bench-scale validation of a hybrid membrane-AOP system

Paola Calza[1], Federico Cristaudo[1], Delia Revelli[2], Vittorio Boffa[3], Debora Fabbri[1]
[1]Dipto di Chimica, Università di Torino, Italy; [2]Azienda Agricola San Biagio, San Biagio, Italy; [3]Aalborg University, Denmark

Aquaculture is a rapidly expanding sector demanding sustainable water management strategies to mitigate the release of contaminants. The feasibility of an integrated treatment sequence combining novel ceramic membranes and advanced oxidation processes (AOPs) for water reuse was explored. A nanostructured ceramic membrane coated with ZIF-8@ SiO_2-ZrO_2 gel core-shell nanoparticles was successfully upscaled from laboratory development to a real-scale multichannel module (1179 mm length, 25 mm diameter) and validated at bench scale using real aquaculture effluents spiked with sulfamethoxazole and carbamazepine as model micropollutants. The ceramic membrane exhibited high permeability, mechanical robustness, and chemical resistance, enabling direct treatment of fish farm effluents and effective protection of downstream technologies. While showing moderate selectivity toward micropollutants, the membrane proved to be well suited as a pretreatment step for nanofiltration. Integration with NF90 nanofiltration enabled efficient concentration of pollutants into the retentate, subsequently treated by photocatalysis using a co-doped P-In-C_3N_4 catalyst. The tailored co-doping enhanced charge separation and reactive species generation, enabling complete removal of contaminants under simulated solar irradiation despite the complex retentate matrix.
The innovation of the proposed approach lies in two complementary steps: first, the application of a MOF-based ceramic coating on a real-scale membrane module can be used as a unique pretreatment for complex aquaculture effluents, even under spiked conditions, prior to nanofiltration; second, the integration of photocatalysis directly addresses the issue of contaminant accumulation in the concentrated retentate, allowing efficient treatment of a reduced-volume stream that would otherwise be problematic for AOPs.



(A) Schematic representation of the bench-scale setup and pictures of (B) the feed tank, (C) the treated aquaculture water, (D) the membrane housing, and (E) the HDI to operate the system.

Acknowledgements: This research was funded by the European Union under the Marie Skłodowska-Curie Actions (MSCA) – Research and Innovation Staff Exchange Suswater (grant agreement No 101007578).

EES - D3 - P07
Composition and efficacy of essential oils in suppressing potato sprouting

Klaudia Jakubowska, Julia Kamińska, Paweł Gulski, Gabriela Kuźma, Kazimierz Warmiński
University of Warmia and Mazury in Olsztyn, Poland

Potatoes are one of the most commonly consumed foods in the world, but their natural tendency to sprout during storage poses a significant technological problem. Extending the storage life of potatoes involves controlling temperature and using sprout inhibitors. One of the most commonly used compounds was chlorpropham (CIPC). However, growing concerns about its harmfulness have led to the withdrawal of CIPC in the European Union (EU) and the search for alternative solutions. The most interesting alternatives are natural essential oils (EOs)[1]. The EO best described in the scientific literature is caraway EO, which contains carvone. Biopreparations containing carvone based on spearmint EO are already approved for marketing in the EU.
In our studies, we have shown that other EOs have a suppressive effect on potato sprouts, including coriander seeds (*Coriandrum sativum* L.), dill seeds (*Anethum graveolens* L.), tansy (*Tanacetum vulgare* L.) and thuja (*Thuja occidentalis* L.). EOs were produced by hydrodistillation in a Deryng apparatus (10 dm^3). The chemical composition of EOs was determined by GC-MS using a Schimadzu QP-2020NX system. A correlation was found between the content of carvone, phellandrene, thujone and the bioactivity of EOs. However, a question to be addressed in future studies will be to determine the safety of using EOs containing harmful thujone (thuja, tansy). EOs from dill and coriander are safer, as is caraway oil.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P08

Comparison of the yield and chemical composition of essential oils from the seeds, leaves and straw of *Apiaceae* plants

Julia Kamińska, Klaudia Jakubowska, Gabriela Kuźma, Paweł Gulski, Kazimierz Warmiński
University of Warmia and Mazury in Olsztyn, Poland

Essential oils (EOs) are products derived from plant raw materials, obtained by steam distillation, hydrodistillation, and less frequently by pressing and dry distillation. EOs generally consist of mixtures of terpenoids, phenylpropanoids, esters, aldehydes, and alcohols. The components of EOs are very interesting from an application point of view. EOs have unique properties (volatility, pleasant smell, bioactivity), which make them widely used in industry, medicine and agriculture[1,2].

The aim of the study was to compare the chemical composition of EOs produced from different parts of plants (seeds, leaves and waste straw) of species from the *Apiaceae* family: dill, fennel, caraway, coriander, celery, parsley. EOs were produced by hydrodistillation in Deryng apparatus (10 dm^3). The chemical profile of EOs was determined by GC-MS using a Schimadzu QP-2020NX system. The results of our study revealed that the highest EO yield was obtained from seeds, especially caraway (2.66% v/m) and dill (1.90%). In the case of EOs from leaves, celery had the highest yield (0.26%). This is important because celery leaves are often a by-product of horticulture. Dill straw contained the least amount of EO (only 0.10%). *Apiaceae* EOs were characterised by a diverse chemical composition. For example, the dominant components of dill EO were α-phellandrene, β-cymene and D-limonene, while caraway EO contained D-carvone and D-limonene. The straw, leaves and seeds of a given species had a similar EO chemical profile.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P09
Contact electrification of some organic powders with fused aromatic ring structures

Mahnam Ebadi[1], Niloofar Kamyar[1], Bilge Baytekin[1]
[1]Bilkent University, Turkey

Static charge accumulation on insulating surfaces causes a variety of issues in many industries. The mechanism of charge accumulation via contact and subsequent charge dissipation has been studied since ancient times, yet it remains poorly understood. The static charge-related problems are even more pronounced when powder materials are involved.
In this study, our objective is to provide a more systematic perspective on the charging of organic material powders. The basic question is whether the chemical structure is a dominant factor in the triboelectrification of insulating powders. Therefore, simple and common aromatic powders with varying numbers of aromatic rings are analyzed according to their charging propensities under identical conditions. Also, we studied the impact of the type, number, and position of certain functional groups in the molecular structure on the material's triboelectrification.
We ground the powder materials in an agate mortar with a steel and agate pestle to charge them. An electrostatic voltmeter was then used to measure the electric potential developed on the powder. The results show sign and magnitude of the electrostatic potential seemed to be related to the number of fused aromatic rings. Additionally, powders of some compounds bearing functional groups, such as nitro or carboxyl, were negatively charged, while powders with molecular structures bearing a methyl group were positively charged. We studied particle morphology via SEM and crystallinity via XRD analysis to determine whether these material attributes change before and after grinding and whether these changes make a decisive contribution to the electrification outcome. Our results show that, as hypothesized, the molecular structure is the largest influencer of powder triboelectrification. We believe that a fundamental understanding of the physical properties and chemical structure can help solve future powder charging-related problems.

EES - D3 - P10

Directional charge transport in donor–acceptor covalent organic frameworks for enhanced photocatalytic H_2O_2 production

Muzammil Hussain[1], Zhongliang Wen[1], Titus de Haas[2], Pascal Van Der Voort[1]
[1]COMOC—Center for Ordered Materials, Organometallics and Catalysis, Dept. of Chemistry, Ghent University, Belgium; [2]Center for Molecular Modeling (CMM), Ghent University, Belgium

The development of efficient photocatalysts requires the optimization of several interrelated factors, including light absorption, exciton generation and dissociation, charge transport, band alignment with redox reactions, and surface properties. Donor–acceptor (D–A) two-dimensional covalent organic frameworks (COFs) are promising photocatalysts due to their ability to facilitate exciton separation. However, the preferred direction of charge transport (whether within the plane or along the out-of-plane (z) direction) and its role in catalytic performance remain unclear. Here, we examine charge-transfer pathways in three structurally comparable D–A COFs (TAPD–TT, TAPD–TFTA, and TAPD–TA) constructed from the electron-rich knot N,N,N′,N′-tetrakis(4-aminophenyl)-1,4-phenylenediamine (TAPD) and acceptor linkers with systematically varied electron densities. Using a combination of experimental techniques and density functional theory (DFT), we correlate photophysical behavior with photocatalytic H_2O_2 production.

Exciton separation occurs predominantly within the two-dimensional planes through the D–A effect, with comparable separation efficiencies across all three COFs, indicating that pronounced donor–acceptor electron density differences are not strictly required. Hole transport is efficient in all directions, showing a clear preference for in-plane motion with effective masses between 0.5 and 1.4 m_e. In contrast, electrons are heavy in the xy-plane, with effective masses near 6 m_e. Along the z-direction, however, TAPD–TT exhibits a substantially lower electron effective mass (~2.5 m_e), markedly smaller than those of TAPD–TFTA and TAPD–TA. This enhanced out-of-plane transport in TAPD–TT arises from tight vertical stacking of TT acceptor units, which maximizes π–π overlap and enables efficient interlayer electron mobility. The resulting directional charge transport directly correlates with superior photocurrent generation and the highest H_2O_2 production rate.

These findings establish structure–charge transport–activity relationships and highlight directional electron mobility as a decisive design parameter for high-performance photocatalytic COFs.

Acknowledgements: PVDV, MH and TdH acknowledge the FWO Vlaanderen and the iBOF financing (COFLIGHT, 01IB7625).

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EES - D3 - P11
Inhibition of seed germination by selected essential oils: Relationship with chemical composition

Paweł Gulski, Gabriela Kuźma, Klaudia Jakubowska, Julia Kamińska, Kazimierz Warmiński
University of Warmia and Mazury in Olsztyn, Poland

Essential oils (EOs) are volatile liquid substances obtained from plant materials through steam distillation. In recent years, EOs have been the subject of interest as potential bioherbicides, which is in line with the idea of bioeconomy and green chemistry[1]. The aim of this study was to determine the chemical composition of EOs obtained from selected plant materials and to evaluate their inhibitory effect on seed germination (phytotoxicity). The research material consisted of: (1) herbs: tansy (*Tanacetum vulgare* L.), Canadian goldenrod (*Solidago canadensis* L.); (2) seeds: dill (*Anethum graveolens* L.), caraway (*Carum carvi* L.), coriander (*Coriandrum sativum* L.); (3) biomass of whole plants: Scots pine (*Pinus sylvestris* L.), thuja (*Thuja occidentalis* L.), Nordmann fir (*Abies nordmanniana* (Steven) Spach). Essential oils were obtained by hydrodistillation in a Deryng apparatus (10 dm^3). The chemical profile was determined by GC-MS using a Schimadzu QP-2020NX system. Biological activity was determined in phytotoxicity tests. The tested EOs were characterized by a very complex chemical composition. Each of them contained at least several dozen volatile organic compounds, and the longer the hydrodistillation was carried out, the higher the number of detected compounds and their molecular weights. The main components were monoterpenoids and sesquiterpenoids. It was shown that most of the tested EOs exhibit allelopathic activity. Some of them can potentially be used as bioherbicides, especially those from thuja, coriander, dill, and tansy.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P12

Predictive chemometric modeling of molecular transport in functional organic solvent nanofiltration membranes

Lukka Thuyavan Yogarathinam, Abdul Waheed
Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum and Minerals, Saudi-Arabia

Organic solvent nanofiltration (OSN) membranes have widespread industrial applications. In this study, ensemble machine learning (ML) coupled with chemometric modeling was applied to functionalized polyacrylonitrile (PAN)–supported poly(piperazine-amide) thin-film composite (TFC) membranes to enable data-driven prediction of OSN performance. Diamines such as ethylenediamine (EDA) and hydrazine (Hz) were cross-linked with PAN membranes to produce functionalized supports, and their impact on TFC membrane performance for OSN was systematically investigated. Membrane characterization confirmed that diamine functionalization enhanced poly(piperazine-amide) formation, as evidenced by ATR-FTIR and surface charge analyses. The EDA-cross-linked PAN-supported TFC membrane exhibited minimal solvent swelling, while the hydrazine-modified TFC membrane displayed pronounced hydrophilic characteristics. EDA-TFC and Hz-TFC membranes enhanced polar and aromatic solvent transport through specific hydrogen-bonding, dipolar, and π–π interactions governed by solvent solubility, viscosity, and molecular size. Dye separation experiments using Rose Bengal (RB), Congo Red (CR), Eriochrome Black T (EBT), and Methylene Blue (MB) confirmed that solvent transport and selectivity are strongly influenced by diamine-modified PAN–TFC support chemistry. The EDA-TFC membrane achieved the best balance between flux and rejection, whereas the Hz-TFC membrane delivered higher organophilic flux but with reduced selectivity toward cationic dyes. Accurate prediction of solute transport in OSN is essential for industrial scale-up due to complex solvent and solute–membrane interactions. However, the Spiegler–Kedem framework, while mechanistically informative, is limited by its reliance on constant transport parameters across diverse systems. Principal component analysis (PCA) revealed clear grouping of transport- and interaction-related descriptors, with solvent affinity dominating PC1 and steric and surface effects (molecular size, CN-index, contact angle) defining PC2, in agreement with correlation trends. Among Gaussian process regression (GPR) models, the comprehensive C1 descriptor set delivered near-perfect predictive accuracy (R2 test = 0.986, RMSE test = 0.703)., outperforming reduced descriptor by effectively capturing coupled transport, steric, and surface-chemistry effects governing dye rejection.

Keywords: Gaussian process regression; Machine learning; Organic solvent nanofiltration (OSN); Thin-film composite (TFC).

EES - D3 - P13

Sunlight-powered reverse water gas shift reaction catalysed by plasmonic Au/CeO_{2-x}: The impact of size, metal loading and oxygen vacancies on the catalytic performance

Romy van Geijn[1,2,3], Jordi Volders[1,2,3,5], Esmee Roman[1,2,3], Sander Bossier[4], Sander Stullens[1,2,3], Bjorn Joos[1,2,3], Thomas Vranken[1,2,3], Francesc Sastre[5], Jan D'Haen[2], Ken Elen[1,2,3], Marcel A. Verheijen[6,7], Daniel Mann[1,5], Pegie Cool[4], An Hardy[1,2,3], Marlies K. Van Bael[1,2,3] and Pascal Buskens[1,5]

[1]Institute for Materials Research (imo-imomec), DESINe Group, Hasselt University, Belgium; [2]IMOMEC Associated Laboratory, IMEC vzw, Belgium; [3]EnergyVille, Belgium; [4]Laboratory of Adsorption and Catalysis, Dept. of Chemistry, University of Antwerp, Belgium; [5]The Netherlands Organisation for Applied Scientific Research (TNO), The Netherlands; [6]Dept. of Applied Physics, Eindhoven University of Technology, The Netherlands; [7]Eurofins Materials Science, The Netherlands

The reverse water gas shift (rWGS, eq. 1) reaction is an attractive pathway for CO_2-to-CO conversion; however, it is endothermic and directly competes with the exothermic Sabatier methanation reaction (eq. 2), requiring high temperatures for CO selectivity. Photocatalysis offers a low-temperature alternative.[1,2]

rWGS $\quad CO_2 + H_2 \leftrightarrows CO + H_2O \quad \Delta H_{298K} = +41.2\ \text{kJ mol}^{-1}$ (1)

Sabatier reaction $\quad CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \Delta H_{298K} = -165.0\ \text{kJ mol}^{-1}$ (2)

In this study, we selected Au/CeO_{2-x} as plasmonic catalyst for the sunlight-powered rWGS reaction. A systematic study of the impact of Au particle size and loading on the its catalytic performance has not yet been reported. Furthermore, the influence of oxygen vacancies is unknown. We focus on elucidating the impact of these characteristics on the catalytic performance.

We successfully produced Au/CeO_{2-x} catalysts.[3] Both size of Au and CeO_{2-x} was varied and the Au loading on the CeO_{2-x} surface (Fig. 1). Furthermore, various techniques were applied to tailor the concentration of oxygen vacancies.

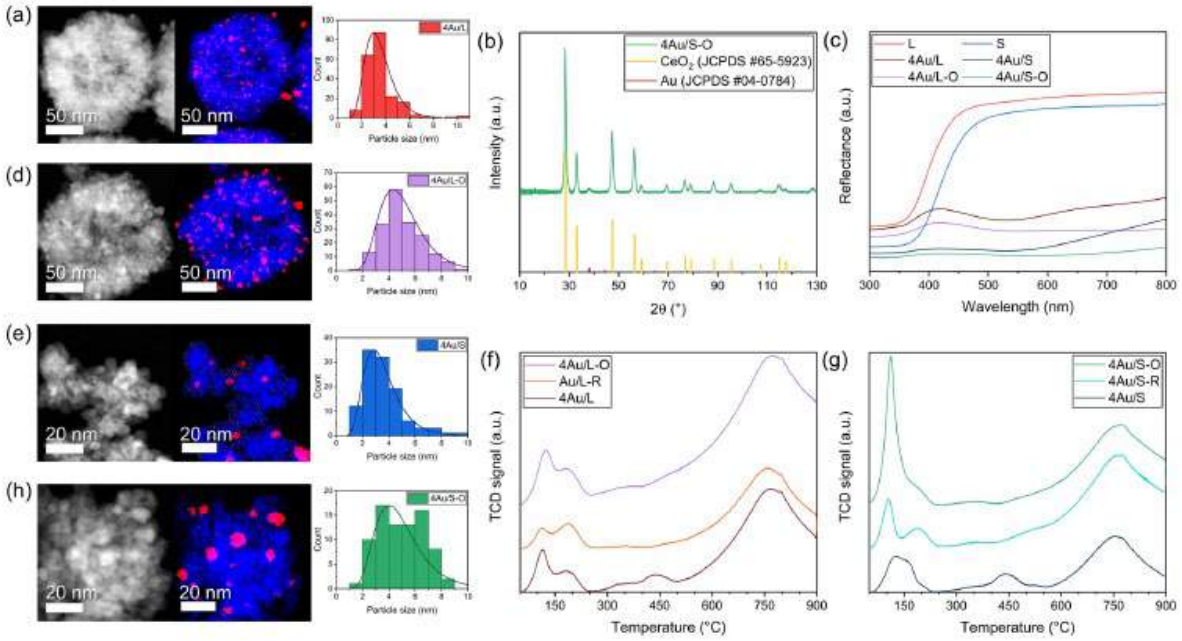

Fig. 1. Representative HAADF-STEM image, EDX mapping in STEM mode and Au particle size distribution from TEM analysis with lognormal fit of various Au/CeO_{2-x} catalysts (a, d, e, h). CeO_{2-x} is coloured blue and Au is coloured red in EDX mapping, lower magnification shown for (a) and (d) to illustrate CeO_{2-x} size particle difference. (b) XRD diffractogram of 4Au/S-O. (c) Reflective diffuse UV-vis spectra of various (Au/)CeO_{2-x} catalysts; graphs have been stacked for visual clarity. H_2-TPR profiles of (f, g) various Au/CeO_{2-x} catalysts; graphs have been stacked for visual clarity.[3]

By assessing the performance of the catalysts, we obtained following key findings: (1) Upon illumination, all catalysts produced CO with a selectivity of ≥98% at low catalyst surface temperatures; (2) The CO production rate increased exponentially with the irradiance, confirming photothermal heating; (3) In dark, all catalysts formed CH_4

instead of CO, indicating that plasmon-induced desorption of CO plays a vital role; (4) The activity depends linearly on the accessible interfacial area between CeO_{2-x} and Au, which is in line with an associative reaction mechanism.[4] Currently, we are focusing on preparing catalysts with a high loading of small Au nanoparticles to study the impact of interparticle distance. To achieve high loadings of small Au nanoparticles, we designed a new Au deposition step involving Sn-mediated nucleation. To date, we have successfully prepared Au/CeO_{2-x} catalysts using this technique (Fig. 2). We are currently optimizing this synthesis procedure and assessing the performance of these catalysts.

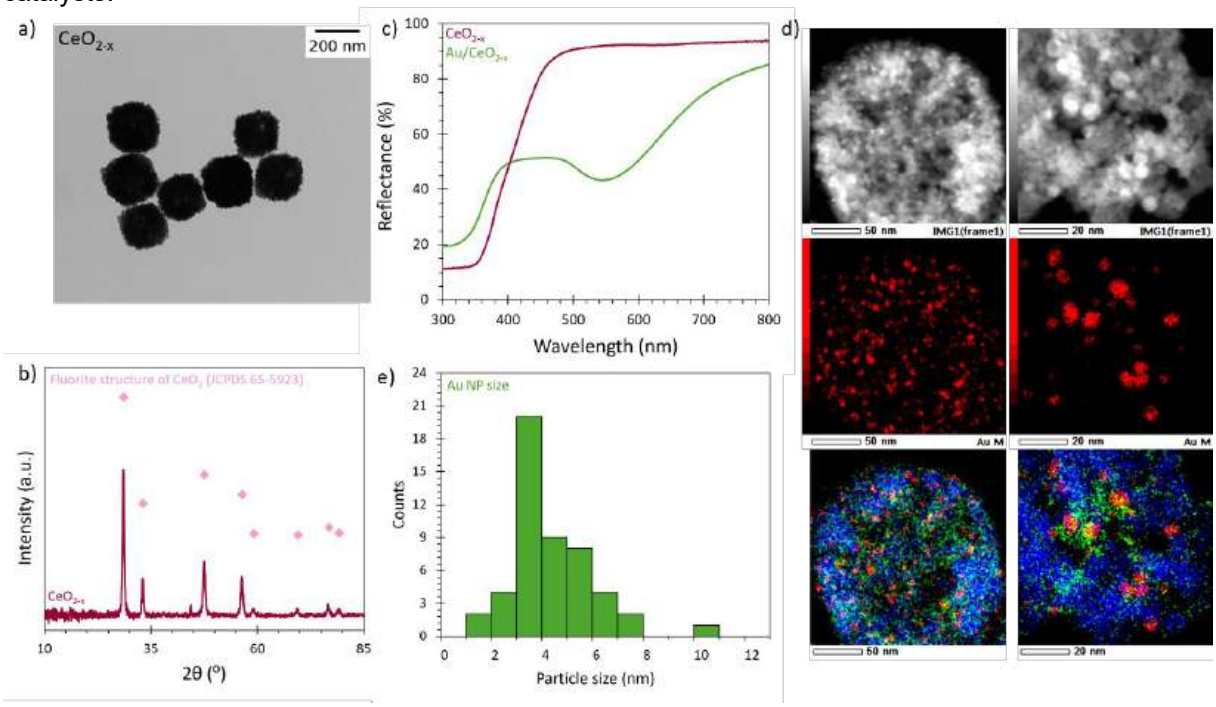

Fig. 2. (a) TEM image of CeO_{2-x} particles, with an average particle radius of 121.1 ± 1.13 nm calculated from multiple images. (b) XRD diffractogram of CeO_{2-x}; the crystallite size, calculated using the Scherrer equation from the (111) diffraction peak at $2\theta \approx 28.5°$, is 19.75 ± 1.72 nm. (c) Diffuse-reflectance UV-Vis spectra of CeO_{2-x} and Au/CeO_{2-x}. (d) Representative HAADF-STEM image and corresponding STEM-EDX elemental maps of Au/CeO_{2-x} with a theoretical gold loading of 5.5 wt%, showing Ce in blue, Sn in green, and Au in red. (e) Histogram of the gold nanoparticle size distribution for Au on CeO_{2-x}, determined from STEM-EDX analysis, with an average particle size of 4.38 ± 1.69 nm.

Acknowledgements: This work received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 101015960 (SPOTLIGHT), the EC Interreg Flanders-The Netherlands project FOTON and the Research Foundation Flanders (FWO-Vlaanderen) under project No. G0A4924N (PICaSSo). Solliance and the Dutch province of Noord-Brabant are acknowledged for funding the TEM facility.

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EES - D3 - P14
Safe and sustainable materials as adsorbents for emerging pollutants

Carla Rizzo[1,*] , Antonio Mineo[2], Sara Amata[1], Giorgio Mannina[2], Antonio Palumbo Piccionello[1]
[1]Dept. of Biological, Chemical and Pharmaceutical Sciences and Technologies, Palermo University, Italy; [2]Engineering Dept., Palermo University, Italy

The increasing demand of polymeric materials in combination to the interest in preventing environmental pollution recently brought to the design and synthesis of polymeric materials from sustainable feedstocks. Several efforts have been devoted to the synthesis of bio-based polymers via ring-opening metathesis polymerization from epoxidized soybean oil and its copolymerization.[1,2] While the polymerization of the crude soybean oil is less investigated, in this framework an easy conversion of soybean oil in a durable and chemical degradable material has been recently reported.[3]
The bio-polymer can be efficiently applied for wastewater pollutant removal such as dyes, oil and halogenated solvents. However, since December 2024, wastewater treatment has been subject to new regulations (namely, Directive EU. 3019/2024), prompted by the systematic detection of emerging pollutants (microplastics, perfluoroalkyl substances (PFAS), pharmaceutically active compounds (PhACs)). For this reason, the research of new materials able to trap emerging pollutants is urgent.
In this framework, the soybean-oil-derived bio-based polymer mixed with zeolite was evaluated also as a sustainable adsorbent for the removal of an antibiotic, such as doxycycline (DOX), from treated wastewater. Batch tests with a 50:50 mixture of biopolymer and zeolite at initial DOX concentrations of 2.5–7.5 mg L^{-1} achieved 50–60% removal at 2.5–5 mg L^{-1} and nearly complete (≈99%) removal at 7.5 mg L^{-1} after 48 h. Pilot columns packed with the same material treated 100 L of spiked tertiary effluent (1 L h^{-1} for 4 days), exhibiting S-shaped breakthrough curves and sustained antibiotic retention under realistic hydraulic conditions, with faster exhaustion at higher influent loads. Regeneration tests identified 2-methyl-tetrahydrofuran as the most effective solvent for DOX desorption that allows the recyclability of the adsorbent for further adsorption cycles. The results demonstrate the technical feasibility of this regenerable, bio-based material as a candidate adsorbent for conventional and quaternary treatment of urban wastewater.

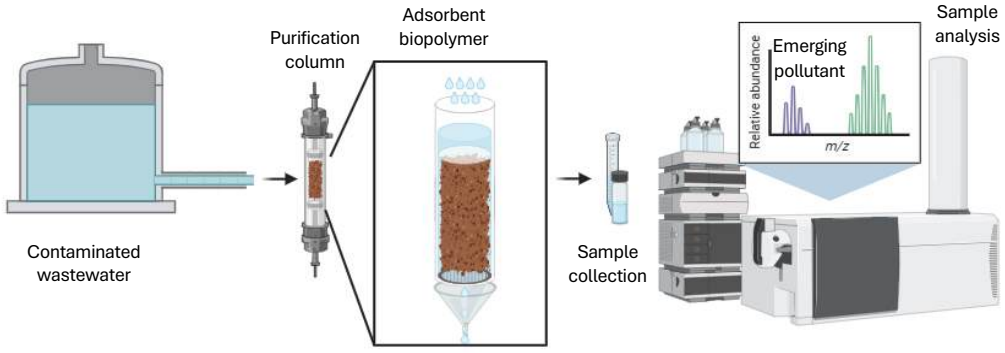

Fig.1. Schematic representation of the pilot scale experimental set-up in which the biopolymer is used as adsorbent material.

This work was funded with University of Palermo Funds, EUROSTART 2025 Call, research project “SAFE - Sustainable Adsorption with Functionalized-biopolymers for Emerging pollutants”, PRJ-2195.

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EES - D3 - P15
Understanding structural and electrochemical degradation in Li-rich cathodes

Alyssa Mancini*[1, 2,] Eleonora de Santis [2], Giovanni Battista Appetecchi[2], Sergio Brutti[1], Arcangelo Celeste[1], Laura Silvestri[2]
[1]Dept. of Chemistry, University of Rome Sapienza, Roma, Italy; [2]Dept. of Energy Technologies and Renewable Sources, ENEA C.R. Casaccia, Roma, Italy

Li-rich layered oxides (LRLOs) are promising high-capacity cathode materials for lithium-ion batteries, offering capacities above 200 mAh g^{-1} through combined cationic and anionic redox activity [1]. Their application is limited by structural and electrochemical instabilities, including transition metal redistribution, microstructural damage, and voltage decay [2]. In this study, a Co-free LRLO with composition $Li_{1.18}Mn_{0.52}Ni_{0.3}O_2$ was synthesized via a solid-state route combining ball milling and calcination and tested in lithium cells using both a conventional carbonate-based electrolyte and an ionic liquid-based electrolyte. Ex situ synchrotron X-ray fluorescence (XRF) 2D imaging at multiple length scales was employed to probe the spatial distribution of transition metals within electrode particles. The measurements show that cycling in the carbonate-based electrolyte induces manganese redistribution and localized heterogeneities, associated with early microstructural changes [3], whereas the ionic liquid electrolyte preserves a more uniform distribution of transition metals and a more intact electrode structure. These findings indicate that manganese migration contributes significantly to the structural and electrochemical degradation of Co-free LRLOs and that electrolyte composition can influence the extent of these effects. By linking transition metal distribution to cycling behavior, this study provides direct experimental insight into degradation mechanisms in Li-rich cathodes, supporting the development of strategies to improve their stability and lifetime.

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EES - D3 - P16
Controlled incorporation of monoboc-protected amines in polyamide thin-film composite membranes

Tauqir Ahmad[1], Abdul Waheed[1]
[1]Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia

Thin-film composite polyamide membranes were fabricated via interfacial polymerization with controlled incorporation of ethylenediamine monoboc (EDAM) as a functional amine modifier. By varying the proportion of EDAM during membrane formation, a series of chemically tailored membranes with distinct structural and surface characteristics were obtained. The membranes were systematically characterized using spectroscopic, microscopic, thermal, and surface analyses to confirm successful modification and to evaluate changes in morphology, chemical composition, wettability, and stability. The influence of amine modulation on membrane transport behavior was further examined under pressure-driven filtration conditions. This study demonstrates a versatile strategy for fine-tuning polyamide membrane properties through controlled amine chemistry, offering a scalable route toward next-generation membranes with improved performance and tunable physicochemical features for water and separation applications.

We would like to acknowledge the support provided by the IRCMWS at KFUPM and all the universities involved in this work. The authors would like to acknowledge support from INMW2422.

EES - D3 - P17
Recovery and regeneration of cathode materials via direct recycling

Myriam D'Alù[1,2], Emanuele Serra[1], Silvano Del Gobbo[1], Antonino Cataldo[1], Pier Paolo Prosini[1], Sergio Brutti[2], Priscilla Reale[1], Rocco Cancelliere[1], Laura Silvestri[1]
[1]ENEA, Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Rome, Italy; [2]University Sapienza of Rome, Rome, Italy

The rapid expansion of electric vehicles and portable electronics is driving a sharp increase in lithium-ion battery production, intensifying pressure on critical raw materials (CRMs) and resulting in a growing volume of end-of-life batteries that still contain significant amounts of valuable metals[1]. Developing sustainable recycling strategies capable of closing the loop is therefore a key challenge for the battery value chain.
Direct recycling has gained increasing attention as it aims to recover cathode materials while preserving their original structure and functionality. By avoiding complete elemental breakdown, this strategy has the potential to reduce energy consumption and environmental impact compared to conventional recycling routes.
Here, we investigate the recovery and regeneration of NMC materials from spent lithium-ion cells. Different routes were explored to separate the active material from the current collector, including mechanical and solvent-based delamination methods. All approaches enabled effective recovery of the cathode powder, although typical degradation and processing related impurities were observed in the recovered material. Regeneration of the spent cathode was carried out through solid-state relithiation designed to restore stoichiometry and structural order. Chemical-physical characterization confirmed the re-establishment of the layered structure while the electrochemical characterization demonstrated that the regenerated material recovered a substantial fraction of its original performance.
Overall, this study demonstrates the effectiveness of direct recycling for regenerating cathode materials from end-of-life LIBs[2]. The results highlight the potential of this approach to support a more circular battery economy by reducing waste, lowering environmental impact, and decreasing dependence on critical raw material supply.

The authors acknowledge IPCEI project European Battery Innovation (EuBatIn) funded by Ministero dell'ambiente e della sicurezza energetica.

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EES - D3 - P18

Advanced sorption-based recovery of rare-earth elements from secondary aqueous streams: A contribution to EU strategic autonomy and circular critical raw materials

Eduarda Pereira[1]*, Joana Sousa[1], Daniela S. Tavares[1,2], Bruno Henriques[1], Filipe L.S. Monteiro[1], Zhi Lin[3], João Rocha[3]

[1]LAQV-REQUIMTE, University of Aveiro, Portugal; [2]LCA – Central Laboratory of Analysis, University of Aveiro, Portugal; [3]CICECO, Dept. of Chemistry, University of Aveiro, Portugal

The accelerating deployment of low-carbon and digital technologies has driven unprecedented demand for rare-earth elements(REEs), exposing the European Union's reliance on imports and primary mining, mainly outside Europe. This reliance poses risks to supply security and sustainability. In alignment with the EU Critical Raw Materials Act, EU Green Deal, and Horizon Europe strategic autonomy goals, efficient recovery of REEs from secondary sources is essential to foster circular critical raw material value chains and reduce environmental burdens[1,2].

Here we investigate a microporous niobium–iron silicate ($Na_{2.9}(Nb_{1.55}Fe_{0.45})_2Si_2O_{10}\cdot xH_2O$) as a sorbent for REEs removal from complex aqueous matrices, including spiked mineral water and simulated electronic waste leachates from permanent magnets and phosphors. Using Response Surface Methodology to optimise pH, initial REE concentration, and sorbent dosage, we demonstrate effective removal across realistic conditions.

Under optimised conditions (pH 4; 180 mg/L sorbent; 2 µmol/L REEs), removal efficiencies exceeded 80% for neodymium (Nd) and 60% for yttrium (Y) in mineral water within 6h. In e-waste solutions, both Nd and Y were removed at >95% efficiency at 5–10 µmol/L. Kinetic modelling indicates chemisorption-dominated uptake, with distinct behaviours consistent with heterogeneous sorption sites and ion-exchange processes.

These results position this sorbent as promising candidates for scalable, non-extractive REE recovery from secondary aqueous streams, advancing EU objectives to strengthen critical raw material resilience and sustainability[2,3].

This work is support from national funds (FCT/MCTES through the CICECO-Aveiro Institute of Materials (UIDB/50011/2020 & UIDP/50011/2020), and REQUIMTE (UID/50006 – Laboratório Associado para a Química Verde – Tecnologias e Processos Limpos). This work is funded by COMPETE2030-FEDER-00847800.

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EES - D3 - P19
Chemical compositions, stability and insecticidal activities of some essential oil emulsions

Gabriela Kuźma, Paweł Gulski, Julia Kamińska, Klaudia Jakubowska, Kazimierz Warmiński
University of Warmia and Mazury in Olsztyn, Poland

Essential oils (EOs) generally consist of mixtures of terpenoids, phenylpropanoids, and other classes of volatile organic compounds. These compounds are very interesting from a scientific and application point of view. For this reason, they are used in the production of flavors, perfumes, cosmetics, repellents, and even medicines and biopesticides[1]. Currently, biopesticides based on EOs from orange, spearmint, and tea tree are already registered on the EU pesticide market.
The aim of our research was to investigate the chemical composition, stability, and insecticidal activity of oil/water emulsions produced from EOs. EOs were produced from the seeds of *Apiaceae* plants: dill (*Anethum graveolens* L.), fennel (*Foeniculum vulgare* Mill.), caraway (*Carum carvi* L.), coriander (*Coriandrum sativum* L.) and biomass from selected coniferous trees. The emulsions were produced from EOs, surfactants (Tween, saponin) and water. The chemical composition of EOs and emulsions was determined using GC-MS. The stability of emulsions was assessed using the turbidimetric method. Insecticidal activity was determined in toxicity tests using *Tenebrio molitor* L. larvae. Based on the tests, it was shown that monoterpenes were the dominant compounds in EOs. Emulsions with EOs from *Apiaceae* seeds showed the best insecticidal efficacy (contact action). The respiratory action of EOs varied, with coriander EO showing the best efficacy. The results of our research show that EOs can be a source of promising bioactive compounds for the production of bioinsecticides.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P20
Gold “self-leaching” in chloride-rich media

Oussama Djorf[1], Fousséni Soma[2], Moussa Bougouma[2], Emmanuel Muragijimana[1], Thomas Doneux[1]
[1]Chemistry of Surfaces, Interfaces and Nanomaterials (ChemSIN), Université Libre de Bruxelles, Belgium; [2]Laboratoire de Chimie Analytique, de Physique Spatiale et Energétique (L@CAPSE), Université Norbert ZONGO, Burkina Faso

In a technology-driven society, the demand for gold has increased due to its widespread use in advanced technologies. However, increased consumption has raised environmental concerns related to extraction and refining. Conventional methods rely on cyanidation, the dominant hydrometallurgical method, because of its efficiency and selectivity, but its extreme toxicity and long-term persistence present major regulatory challenges. These issues have motivated the development of safer, cyanide-free leaching technologies. Chloride-based leaching systems have emerged as promising alternatives, offering faster dissolution kinetics and improved environmental performance.
In the past few years, unconventional solvents such as ionic liquids and deep eutectic solvents (DES) have been gaining increasing attention in this regard because of their potentially minor environmental impact. Recent work in our laboratory[1] revealed a novel and fundamentally different leaching pathway for gold in the choline chloride-oxalic acid dihydrate (DES) through a comproportionation-driven reaction as shown below, which eliminates the need for external oxidants.

$$AuCl_4^- + 2Au + 2Cl^- \rightleftharpoons 3AuCl_2^-$$

This work demonstrates that the comproportionation reaction can occur in a wide range of chloride-rich systems, including aqueous and non-aqueous solutions, DESs, and ionic liquids, highlighting its versatility. Electrochemical and spectroscopic methods were employed to understand the leaching mechanism and to study the influence of acidity, chloride activity, and solvent viscosity on gold dissolution behaviour. The electrochemical data reveal that gold leaching proceeds under sustained non-equilibrium conditions and is strongly governed by mass-transport limitations rather than by thermodynamic equilibrium[2].
This mechanism enables efficient gold recovery with strong green credentials, highlighting its potential as a sustainable and environmentally benign alternative to conventional cyanide-based gold leaching.

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EES - D3 - P21
High-temperature operation of vacuum tube solar collectors using Ionic liquids

José Javier Delgado-Marín, Imane Moulefera, Jesús León-García, Ignacio Carnerero, Mercedes G. Montalbán, Gloria Víllora
Chemical Engineering Dept., Faculty of Chemistry, CEIR Campus Mare Nostrum (CMN), University of Murcia, Spain

In recent decades, renewable energies have expanded worldwide to replace fossil fuels and mitigate climate change. The European Green Deal has accelerated this transition. Spain's favorable climate makes it ideal for solar technologies, particularly efficient vacuum tube solar thermal collectors operating at high temperatures [1].
This study evaluates the feasibility of replacing water, the conventional heat transfer fluid, with the ionic liquid 1-ethyl-3-methylimidazolium acetate as the working fluid in a vacuum tube solar collector. The primary motivation is to overcome the temperature limitation imposed by the phase change of water at 100 °C, since ionic liquids exhibit negligible vapor pressure and much higher thermal stability, enabling operation in the liquid phase at temperatures well above this threshold.
Experimental tests were carried out under full solar radiation conditions using an evacuated tube collector located at the University of Murcia. The system was first characterized using water and subsequently operated with the ionic liquid, maintaining equivalent operating conditions and several constant flow rates to ensure a reliable comparison. The results demonstrate that the ionic liquid allows outlet temperatures exceeding 120 °C without phase change, whereas water is limited to approximately 90 °C. At low flow rates (1 L min^{-1}), the ionic liquid exhibited significantly higher thermal and exergy performance, reaching exergy values close to 27 kW, compared with about 18 kW for water under optimal conditions.
The lower specific heat, high thermal stability, and extremely low vapor pressure of the ionic liquid result in larger temperature rises and safer operation at elevated temperatures. Overall, the findings confirm that ionic liquids constitute a technically viable and highly promising alternative heat transfer medium for solar thermal systems, particularly for industrial applications requiring high-temperature heat in the liquid phase.

a)

b)

Variable	Water	Ionic liquid
Outlet temperature	>90°C	>120°C
Temperature difference in collector	5-25°C	Up to 70°C
Useful heat adsorbed	18 kW	27 kW
Maximum thermal efficiency	80%	100%
Operation at T>100°C	No, undergoes phase change	Yes, remains in liquid phase
Influence of flow rate	Efficiency decrease at high flow rates	Good efficiency at low flow rates
Thermal stability	Up to 100°C	High thermal stability
Operational safety	Risk of overpressure	Safe
Economic viability	Economical and widely available	High cost

Fig. 3. a) Schematic of vacuum tube solar collector used in the experiments. b) Comparison of water and ionic liquid as thermal solar fluids.

Funding: This work is part of the following research projects: Ref. PID2023-150761OB-C21 funded by MICIU/AEI/10.13039/501100011033 and by FEDER, UE and Ref. 22129-PI-22 funded by the research support program of the Seneca Foundation of Science and Technology of Murcia, Spain. J.J. Delgado-Marín acknowledges support from the *Juan de la Cierva* contract (Ref. JDC2023-052774-I) funded by MICIU/AEI /10.13039/501100011033 and the FSE+.

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EES - D3 - P22

Synthesis-route effects on competing phase formation in $Na_{0.67}Mn_{0.75}Ni_{0.25}O_2$

Arcangelo Celeste[1], Antonino Giarrizzo[1], José M. Silva Ferraz[1], Graziano Di Donato[2,3], Stefano Vecchio Ciprioti[1], Sergio Brutti[1]

[1]Sapienza University of Rome, Italy; [2]Helmholtz Institute Ulm, Germany; [3]Karlsruhe Institute of Technology, Germany

Layered transition metal oxides (LTMOs) are among the most promising cathode materials for sodium-ion batteries, yet their electrochemical performance is strongly influenced by phase competition arising from synthesis conditions.[1-2] In this work, we investigate the effect of synthesis route on the structural evolution and electrochemical behavior of $Na_{0.67}Mn_{0.75}Ni_{0.25}O_2$ prepared via solid-state (SS) reaction and sol-gel (SG) methods. Although both routes target the same nominal stoichiometry, they lead to distinct crystallographic outcomes: the SS route predominantly stabilizes the P2 phase, whereas the SG route favors the formation of a P3 phase. Comprehensive characterization using X-ray diffraction, XANES, EXAFS, scanning electron microscopy, and thermogravimetric differential scanning calorimetry reveals comparable bulk local structures but marked differences in morphology, surface chemistry, and crystallization pathways. Electrochemical testing demonstrates that the P2-SS material exhibits superior cycling stability and rate capability, while the P3-SG sample suffers from rapid capacity fading, attributed to structural rearrangements during repeated sodium insertion/extraction. Thermal analysis further highlights the role of synthesis kinetics in directing phase formation and stability. These results underscore that synthesis methodology, beyond nominal composition, plays a decisive role in determining phase stability and electrochemical performance in sodium layered oxides. Our findings emphasize the necessity of precise control over synthesis parameters to optimize Na-LTMO cathodes for high-performance sodium-ion battery.

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EES - D3 - P23
Matrix dependent photochemical transformation of sulfamethoxazole in natural and managed waters

Manuel Andino[1], Debora Fabbri[1], Davide Vione[1], Paola Calza[1]
[1]Dipto di Chimica, Università di Torino, Italy

The photochemical fate of antibiotics in surface waters is strongly influenced by water matrix composition. Sulfamethoxazole (SMZ) is a widely used antibiotic and is frequently detected in aquatic environments, where its persistence and transformation products may pose ecological risks. In this study, we investigate how variations in water composition influence the degradation and persistence of SMZ under environmentally relevant sunlight conditions.
Photodegradation experiments were conducted in real water matrices collected from diverse geographical and environmental settings. Irradiations were performed using a solar simulator, so enabling the assessment of SMZ transformation under conditions dominated by matrix mediated photochemical processes rather than by direct photolysis of the compound.
Marked differences in SMZ degradation kinetics were observed among the water matrices investigated.
Slower transformation occurred in waters with low dissolved organic carbon (DOC), whereas significantly faster degradation was observed in humic-rich waters with high DOC content. These differences were attributed to matrix composition, particularly DOC concentration and fluorescence characteristics, which influence the formation and reactivity of photochemically produced reactive species. Probe compound experiments and oxygen-controlled irradiations indicate that triplet excited states of dissolved organic matter (^{3}CDOM*) play a key role in SMZ degradation in humic-rich matrices. Matrix-dependent transformation pathways led to the formation of distinct transformation products, including the selective production of a phenolic derivative in humic-rich waters, which is predicted to be more toxic than the parent compound. Overall, this study demonstrates that the environmental fate and risk profile of SMZ cannot be generalized, as they depend critically on sunlight exposure and, in particular, on the chemical composition of the receiving water body.

Acknowledgements: This research was funded by the European Union under the Marie Skłodowska Curie Actions (MSCA) Doctoral Network IN2AQUAS (grant agreement No 101119555) and by Research and Innovation Staff Exchange Suswater (grant agreement No 101007578).

EES - D3 - P24
Deep eutectic solvents-enabled closed and open-loop wastes battery recycling

Daniele Motta[1], Giulia Tedde[1], Cristiana Margarita[2], Stefano Nejrotti[1,3,4], Daria Ballardini, [2] Alessandro Damin[1], Chiara Ferrara[5], Claudia Barolo[1,3,4,6], Matteo Bonomo[1,2,6]
[1]University of Turin, Italy; [2]Sapienza, University of Rome, Italy; [3]Institute of Science, Technology and Sustainability for Ceramics (ISSMC-CNR), Italy; [4]URT_CAMPUS, Dept. of Chemical Sciences and Materials Technologies, CNR, Italy; [5]University of Milan Bicocca, Italy; [6]INSTM - National Inter-University Consortium for Materials Science and Technology, Florence, Italy

Current patterns of energy consumption are closely linked to global warming and climate change. The push toward climate neutrality by 2050 and the transition to a sustainable society depend heavily on harnessing renewable energy, which highlights the pivotal role of batteries in the EU's Green Revolution. In particular, lithium-ion batteries have driven the electronics boom. However, the EU lacks a dependable domestic battery supply chain, with raw materials and production facilities largely located abroad, underscoring the strategic need for recycling to build an alternative, more autonomous supply network. Existing recycling methods fall short on sustainability as they require very high temperatures or toxic solvents and involve energy-intensive steps to recover battery-grade materials.
Here, we create a sustainable recycling route (Figure 1) based on Deep Eutectic Solvents (DES), rethinking the entire supply chain, by a single-stage, energy-efficient regeneration of lithium cobalt oxide (LCO) battery cathodes [1]. In case where battery-grade materials cannot be recovered (e.g. lithium manganese oxide. LMO), we expand the scope toward the production of catalysts for biodiesel synthesis [2].
These innovative approaches promise an almost zero-waste, energy-saving recovery process for battery waste, helping to establish a resilient EU supply chain and positioning the Union at the vanguard of the green transition.

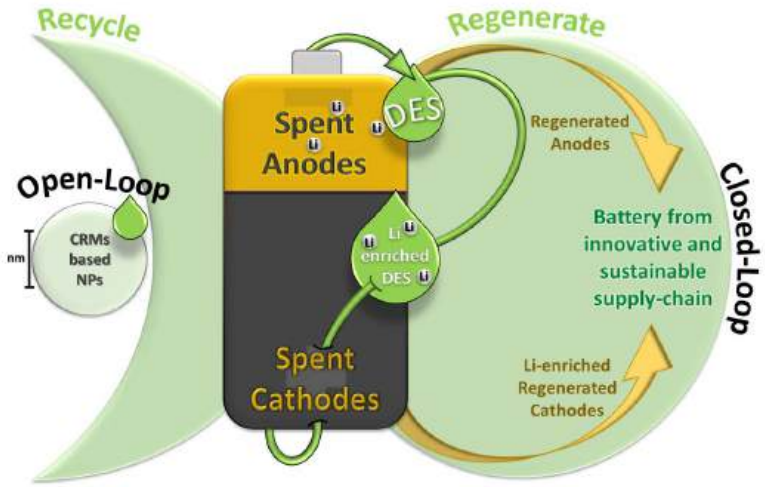

Fig. 4. Our recycling strategy for Spent Electrodes

Acknowledgements: This work was supported by the Fondo Italiano per la Scienza (FIS) under the FIS3 programme, funded by the Ministry of University and Research (Ministero dell'Università e della Ricerca) - Project CUP: [B53C25003870001]. D.M., G.T., S.N., A.D., C.B. and M.B. acknowledge support from the Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023–2027" (CUP D13 C22003520001).

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EES - D3 - P25

Commercial anion exchange membranes for alkaline water electrolysis: Linking performance, stability, and physicochemical properties

Marcelo Cámaras Miguel[1], Kevin Van Daele[1], Nick Daems[1], Tom Breugelmans[1*]
[1]Applied Electrochemistry and Catalysis (ELCAT), University of Antwerp, Belgium

Anion exchange membrane water electrolysis (AEMWE) combines the cost-effectiveness of alkaline systems with the efficiency of polymer electrolyte designs. However, the lack of standardized benchmarking hinders rational material selection and rational AEM design. This study presents a systematic evaluation of nine commercial AEMs (including Fumasep®, PiperION®, Selemion™, Sustainion®, and Xion™) under identical zero-gap conditions.
A comprehensive study of physicochemical properties—including ion exchange capacity (IEC), water uptake, hydration number, and swelling ratio—was conducted to establish structure-property relationships. The analysis reveals that performance is not dictated by IEC alone but by a delicate trade-off between conductivity and dimensional stability. PiperION® 40 µm and Sustainion® X37-50 emerged as top performers, reaching 2 $A \cdot cm^{-2}$ below 2.0 V at 60°C. Their success is attributed to self-supported structures that enable efficient ion transport through optimized hydration channels. In contrast, reinforced membranes exhibited increased ohmic resistance due to the tortuosity introduced by the support matrix, limiting their efficiency despite enhanced mechanical robustness.
Furthermore, ex-situ accelerated stress tests (1 M KOH, 80°C, 168 h) identified critical durability bottlenecks linked to polymer chemistry. The results demonstrated that ether-free backbones (e.g., poly(aryl piperidinium)) offer superior resistance to alkaline hydrolysis compared to aryl-ether based polymers, which suffered significant degradation. Additionally, imidazolium-functionalized membranes showed severe instability at elevated temperatures. These findings provide a vital, comparable dataset to guide the design of next-generation AEMs that simultaneously optimize conductivity, chemical stability, and operational lifetime.

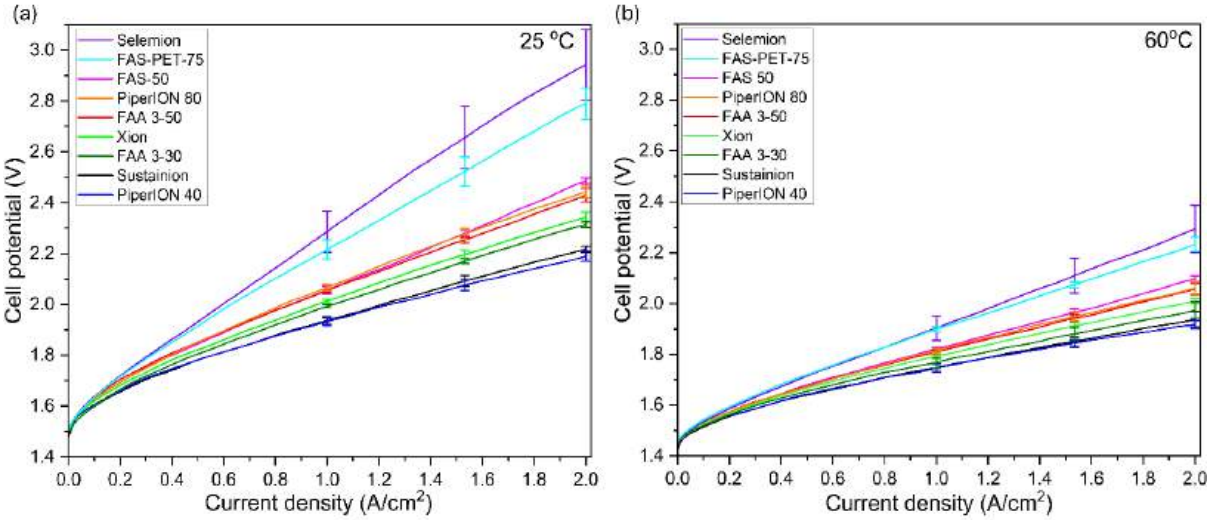

Fig. 1. Polarization curves of nine commercial AEMs measured in a zero-gap AEM water electrolyzer at 25 and 60 °C under identical operating conditions. Error bars represent the standard deviation of triplicate measurements.

This project was funded by the VLAIO ELECZIR project (no HBC.2023.0087)

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EES - D3 - P26
Is atmospheric half-life time of carbon tetrafluoride the same as it was 33 or 47 years ago?

Vladimir Nikiforov
NILU, Norway

Carbon tetrafluoride (CF_4) is perhaps the most stable binary molecule. Nowadays CF4 is regarded as a potent climate gas with an estimated atmospheric lifetime of ≥50,000 years. This value is being reproduced in numerous background documents on climate change, in peer-reviewed papers and in non-scientific publications. The value comes from two independent estimates of Cicerone (1979)[1] and Ravishankara et al. (1993)[2]. Both estimates were based on a postulate that destruction of CF_4 in high-temperature combustion is the major way of its elimination. Naturally, the half-life time of 50,000 years was based on combustion data of late 70-s and early 90-s. Combustion of carbon fuel roughly doubled by 2026. This means the current value is obsolete and must be revised. Furthermore, the assumptions used[1,2] were rather weak and arbitrary. Analytical methods of today allow for inexpensive and accurate quantitation of CF_4. In combination with extensive knowledge on the scale and peculiarities of high-temperature combustion around the globe, it gives an opportunity to obtain an experimental value for atmospheric half-life time of carbon tetrafluoride in high-temperature combustion processes for science-based assessment of its contribution to climate change. In the meantime, the interim value based on the original methods[1,2] in combination with the most recent data for combustion will be presented.

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EES - D3 - P27

Ultra-small Ru and Ni clusters for enhanced CO_2 methanation at ultra-low metal loadings

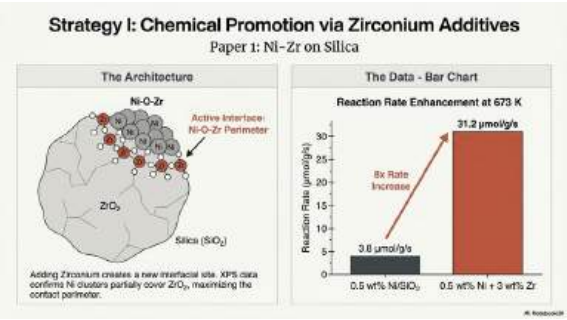
Ching-Shiun Chen[*1,2], Jia Huang Wu[1], Hung-Chi Wu[2]

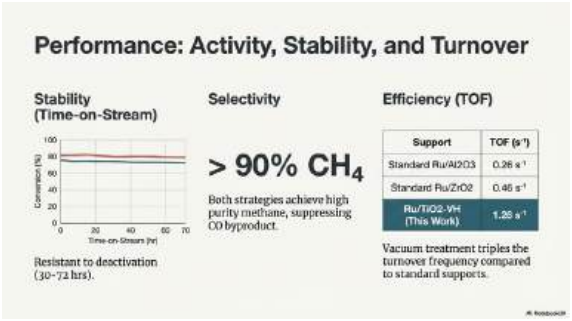
[1]Center for General Education, Chang Gung University, Taiwan; [2]Center for Sustainability and Energy Research Technology, Chang Gung University, Taiwan

The catalytic hydrogenation of carbon dioxide to methane offers a promising route for renewable fuel production and carbon recycling. However, achieving high CO_2 methanation activity and CH_4 selectivity at low metal loadings remains challenging due to limited active site density and insufficient hydrogen activation. This study integrates two catalyst systems—Ru/TiO_2 and $Ni–Zr/SiO_2$—to demonstrate that the formation of ultra-small metal clusters is an effective strategy to enhance CO_2 methanation performance.For Ru/TiO_2 catalysts, a vacuum–hydrogen thermal pretreatment was applied to generate highly dispersed sub-nanometer Ru clusters at very low Ru loadings (0.5–1.0 wt%). This treatment strengthened metal–support interactions, increased surface oxygen vacancies, and promoted the formation of positively charged Ru species. As a result, CO_2 adsorption and hydrogen activation were significantly improved, leading to higher CO_2 conversion and near-complete CH_4 selectivity compared with conventionally prepared catalysts.

The findings demonstrate that atomic-scale Ru clusters can achieve excellent methanation efficiency without requiring high noble-metal content. In the Ni-based system, the introduction of Zr promoters onto low-loading Ni/SiO_2 catalysts (0.5 wt% Ni) created $Ni–ZrO_2$ interfacial sites that markedly enhanced catalytic performance. The Zr additive facilitated CO_2 binding and promoted hydrogen spillover to adjacent Ni clusters, shifting the reaction pathway from CO formation toward direct CH_4 production. These Ni–Zr catalysts exhibited improved CH_4 selectivity and lower activation barriers despite the minimal Ni content.

Overall, the results reveal that precisely engineered small Ru and Ni clusters with optimized metal–support interfaces maximize hydrogen coverage and CO_2 activation, enabling highly efficient CO_2 methanation at ultra-low metal loadings. This cluster-based design provides a sustainable approach for advanced carbon-neutral fuel synthesis.





Acknowledgements: We appreciate the financial support from the National Science and Technology Council (NSTC 114-2113-M-182-001), Chang Gung University (URRPD2Q0021) and Chang-Gung Memorial Hospital (CMRPD5N0022).

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EES - D3 - P28

Optimization of operating parameters in single-stage membrane rotating biological contactor for wastewater treatment

Sharjeel Waqas[1]

[1]Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum and Minerals, Saudi Arabia

Membrane fouling remains a significant challenge that hinders the widespread adoption of membrane separation processes. This study focuses on optimizing the operating parameters of a novel membrane rotating biological contactor (MRBC), an integrated rotating biological contactor (RBC) and membrane filtration system within a bioreactor. The operating parameters (disk rotational speed, hydraulic retention time (HRT), and sludge retention time (SRT)) are optimized using the response surface methodology (RSM). RSM aimed to determine how operating parameters interact to affect filtration performance in the MRBC bioreactor. The results demonstrate that the MRBC achieved removal efficiencies of 84.4% for chemical oxygen demand, 97.1% for ammonium-N, and 43.9% for total nitrogen. RSM resulted in the highest membrane permeability of 456.7 L/m²·h·bar at a disk rotational speed of 35 rpm, 15 h HRT, and 15 days SRT. The proposed model closely matched the experimental data, with a coefficient of determination (R^2) of 0.988. Overall, this study presents a simple, feasible, and proof-of-concept strategy for constructing a compact MRBC design with the potential of minimizing membrane fouling. MRBC is a promising alternative to traditional wastewater treatment methods, offering a compact and efficient process that supports sustainable environmental practices and cleaner production development.

EES - D3 - P29

Matrix-specific partitioning of legacy and emerging PFAS in great tit (*Parus major*) plasma, feathers, and faeces near a fluorochemical hotspot

Oliver Salangad[1], Francesca Cappelli[1], Fabian Simon[1], Jodie Buytaert[2], Lieven Bervoets[2], Thimo Groffen[2], Adrian Covaci[1]

[1]Toxicological Centre, Dept. of Pharmaceutical Sciences, University of Antwerp, Belgium; [2]ECOSPHERE, Dept. of Biology, University of Antwerp, Belgium

Per- and polyfluoroalkyl substances (PFAS) are globally distributed, highly persistent contaminants,[1] yet the matrix-specific fate of emerging and novel PFAS in terrestrial food webs remains poorly understood. This study characterized PFAS occurrence, profiles, and partitioning in great tit (*Parus major*) plasma, feathers, and faeces along a contamination gradient surrounding the 3M fluorochemical plant in Flanders, Belgium. These were integrated with data on highly contaminated soils on the same area (ΣPFAS in soil previously reported up to 118 μg/g)[1] to infer bioavailability, accumulation, and elimination pathways. Targeted and suspect/non-target high-resolution mass spectrometry (SS/NTS-HRMS) revealed 137 individual PFAS from multiple classes. Matrix-dependent differences were evaluated with Kruskal–Wallis tests, with most PFAS showing highly significant partitioning and distinct concentration distributions across soil, plasma, feathers, and faeces.

Plasma was dominated by long-chain PFSAs, 80–100% detection frequencies, and relatively low within-matrix dispersion, consistent with strong protein binding and efficient systemic uptake. Whereas, feathers were enriched in PFESAs and unsaturated sulfonates. Faeces had consistently high detection (>70%) of many long-chain acids and sulfonates. Most of the PFAS showed significant matrix differences, and class-level plasma–soil correlations ranging from $\rho \approx 0.89$ to 0.98 for several legacy and emerging classes, including SF_5-PFSAs, PFESAs, and PFECAs. In contrast, weak class-level plasma–feather correlations indicated decoupling of internal dose and feather burdens. Principal component analyses separated soil, plasma, feathers, and faeces, suggesting combined plasma, feather, and faeces measurements as powerful bioindicators for PFAS biomonitoring at terrestrial hotspots.

Acknowledgements: We are grateful for the funding provided by the University of Antwerp and the Exposome Center of Excellence.

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EES - D3 - P30

Electrochemical dechlorination of PVC for sustainable materials recovery and the synthesis of chlorinated compounds

Hugo Valdés
Depto de Química Orgánica y Química Inorgánica, Instituto de Investigación Química "Andrés M. del Río" (IQAR), Facultad de Farmacia, Universidad de Alcalá, Alcalá de Henares, Madrid, Spain

Poly(vinyl chloride) (PVC) is one of the most widely used plastics and a major contributor to persistent waste streams. Its high chlorine content complicates conventional recycling and frequently leads to downcycling or incineration, with associated environmental impacts. In 2023, Anne J. McNeil and co-workers reported a plasticizer-mediated electro(de)chlorination strategy that enables PVC dechlorination directly from mixed plastic waste.[1] In this paired approach, chlorine equivalents released during dechlorination are leveraged in situ for selective arene chlorination, offering a compelling route to valorize plastic waste through synthetically useful chlorination chemistry. Building on this concept, we developed an electrochemical platform for PVC dechlorination that enables recovery and reuse of released chlorine for benzyl chloride synthesis (Figure 1). Mechanistic evidence[2,3] supports a mediated pathway in which an electrochemical mediator (MedE) is cathodically reduced to MedE•– and subsequently transfers charge to PVC, promoting selective C–Cl cleavage to form PVC• and Cl–. Chloride transport to the anode proved critical, as anodic oxidation generates reactive Cl• species that drive benzylic chlorination of toluene. By comparing divided and undivided cells and implementing biphasic reaction systems, we improved chloride management and benzylic chlorination selectivity while minimizing byproducts. Overall, this work demonstrates a circular "chlorine-loop" electrosynthetic strategy that couples PVC waste remediation with value-added chlorination chemistry, advancing sustainable plastics upcycling.

Fig. 1. Electrochemical dechlorination of PVC coupled to benzyl chloride synthesis.

We acknowledge financial support from Universidad de Alcalá (PIUAH25/CC-074),

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EES - D3 - P31

Rational design of amide-extended tetrahedral linkers for the construction of porous MOFs targeting CO_2 capture

Sharmin Akther Rupa[1*], Robert Davies[1]
[1]Dept. of Chemistry, Imperial College London, UK

Metal-organic frameworks (MOFs) constructed from carboxylate-based linkers continue to demonstrate exceptional potential for applications in gas storage, separation, and catalysis.[1] In this work, we present the design and synthesis of highly branched amide-extended tetrahedral carboxylate linkers, developed by modifying previously established silicon-containing ligands that have been successfully employed within our research group.[2] Incorporating amide functionalities introduces additional sites for hydrogen bonding and guest interactions while enhancing linker rigidity and functionality.[3] These structural features facilitate the formation of robust, three-dimensional MOFs with well-defined porosity and high surface areas.

Several 3D MOFs were synthesized under solvothermal conditions and characterized by single-crystal X-ray diffraction, powder XRD, and spectroscopic techniques. The resulting frameworks display high crystallinity, permanent porosity, and excellent thermal stability. CO_2 uptake studies were performed at 273 and 298 K, revealing significant adsorption capacities consistent with the high surface areas and accessible functional sites of the frameworks.

This work highlights the potential of amide-functionalized derivatives of silicon-based linkers as a versatile platform for the rational design of functional MOFs for CO_2 uptake.

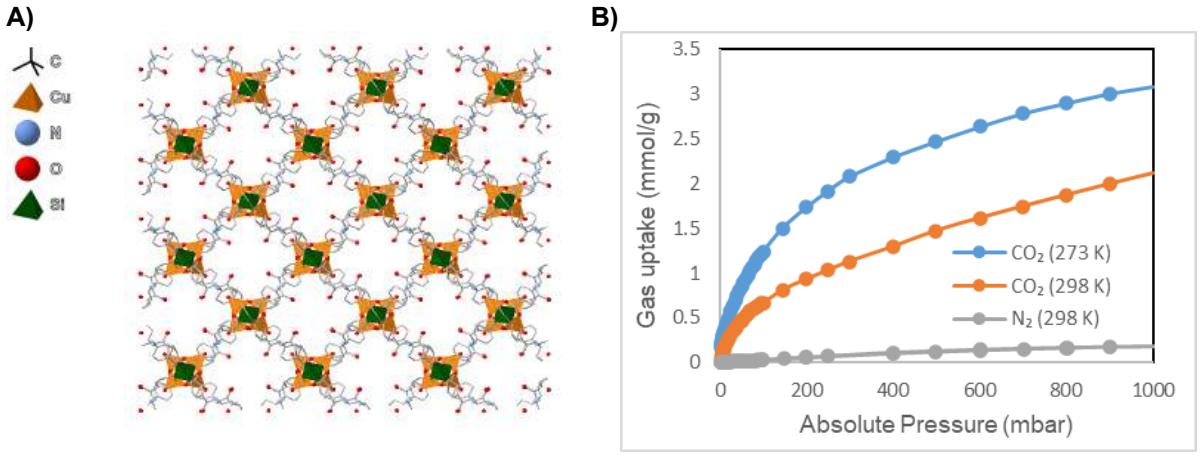

Fig. 1 Single-crystal X-ray diffraction (SXRD) of 3D MOFs A) Cu-MOF using a tetrahedral Si-centred linker B) CO_2 and N_2 uptake studies of the MOFs.

Acknowledgement: The authors gratefully acknowledge the **Commonwealth Scholarship Commission** for funding this research. We also thank **Schlumberger (SLB)** for their support and provision of resources that facilitated this study.

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EES - D3 - P32
Functionalized graphene oxide membranes for high flux nanofiltration

Yasir Abbas[1], Niaz Ali Khan[1,2], Isam H. Aljundi[1,3]
[1]Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum & Minerals, Saudi Arabia; [2]Dept. of Materials Science and Engineering, King Fahd University of Petroleum & Minerals, Saudi Arabia; [3]Chemical Engineering Dept., King Fahd University of Petroleum & Minerals, Saudi Arabia

Graphene oxide (GO) membranes have attracted significant interest for nanofiltration applications due to their tunable interlayer spacing and chemical versatility[1,2,3]. However, pristine GO membranes often suffer from extremely low water permeability (~1 $L.m^{-2}.h^{-1}.bar^{-1}$), which critically limits their practical utility[4]. In this work, we demonstrate a substantial performance breakthrough by functionalizing GO with a covalent organic framework (COF) assembled from the cationic monomer ethidium bromide and 1,3,5-triformylphloroglucinol. The intercalation of the cationic COF within GO nanosheets effectively tunes and stabilizes the interlayer channels, creating well-defined transport pathways for water molecules while simultaneously enhancing electrostatic interactions with target solutes (Figure 1). As a result, the functionalized membranes exhibit an ultrahigh water flux of 73.5 $L.m^{-2}.h^{-1}.bar^{-1}$, over 70-fold higher than pristine GO, while maintaining excellent rejection toward low molecular weight organic compounds. This remarkable synergy arises from the combined effects of (i) improved interlayer spacing uniformity, (ii) increased hydrophilicity and charge-assisted transport, and (iii) strong size- and charge-based selectivity[5,6]. The structural incorporation of the COF within the GO lamellar architecture was unambiguously confirmed by X-ray diffraction, Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy, and electron microscopy, among other techniques, affirming the successful construction of the hybrid framework. Overall, this strategy illustrates a powerful route to overcoming the permeability–selectivity trade-off in GO-based membranes, enabling their deployment for high-efficiency nanofiltration of challenging organic micropollutants. Our findings highlight the potential of rationally designed GO–COF composites as scalable, high-performance membrane materials for next-generation water treatment technologies.

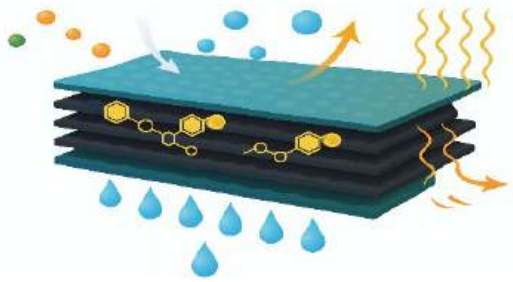

Fig.5. Schematic illustration of EtBr COF-functionalized GO membrane showing enhanced ion sieving and water permeance.

Acknowledgement: The authors would like to acknowledge the support provided by King Fahd University of Petroleum and Minerals, Interdisciplinary Research Center for Membranes & Water Security (project # INMW2512).

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EES - D3 - P33
Oxidative denitrogenation using sustainable carbon nanotubes: Reactive oxygen species

Fernanda F. Roman[1], Adriano Silva[1], Adrian M. T. Silva[2], Joaquim L. Faria[2], Helder Gomes[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal; [2] LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, Portugal

Oxidative denitrogenation (ODN) is a process that allows removing undesired N species from fuels[1]. H_2O_2 is the main oxidant source[1], which should be decomposed into reactive oxygen species by proper catalysts to achieve suitable reaction rates. Another current issue is the accumulation of plastic solid waste (PSW), which can be upcycled into carbon nanotubes (CNTs), thus substituting fossil-derived precursors in the obtention of advanced materials[2]. In this work, CNTs were synthesized from polymers, following the procedures detailed here[2] for POL-OX@NiFe synthesis. The CNT was used as catalyst for ODN of quinoline (QN). QN (in aqueous and oily phases) and H_2O_2 were monitored. tert-butanol and p-benzoquinone were used as indirect probes for $HO^{\bullet}$ and $O_2^{\bullet-}$ (Figure 1). The addition of tert-butanol (50 mM) caused a pronounced decrease in QN oxidation, reducing global removal after 2 h from ca. 90 to ~40%, confirming that $HO^{\bullet}$ are relevant oxidizing species. The addition of p-benzoquinone (10 mM) caused a milder inhibition (QN removal at 2 h of ~66%), suggesting that $O_2^{\bullet-}$ participate as secondary oxidants.

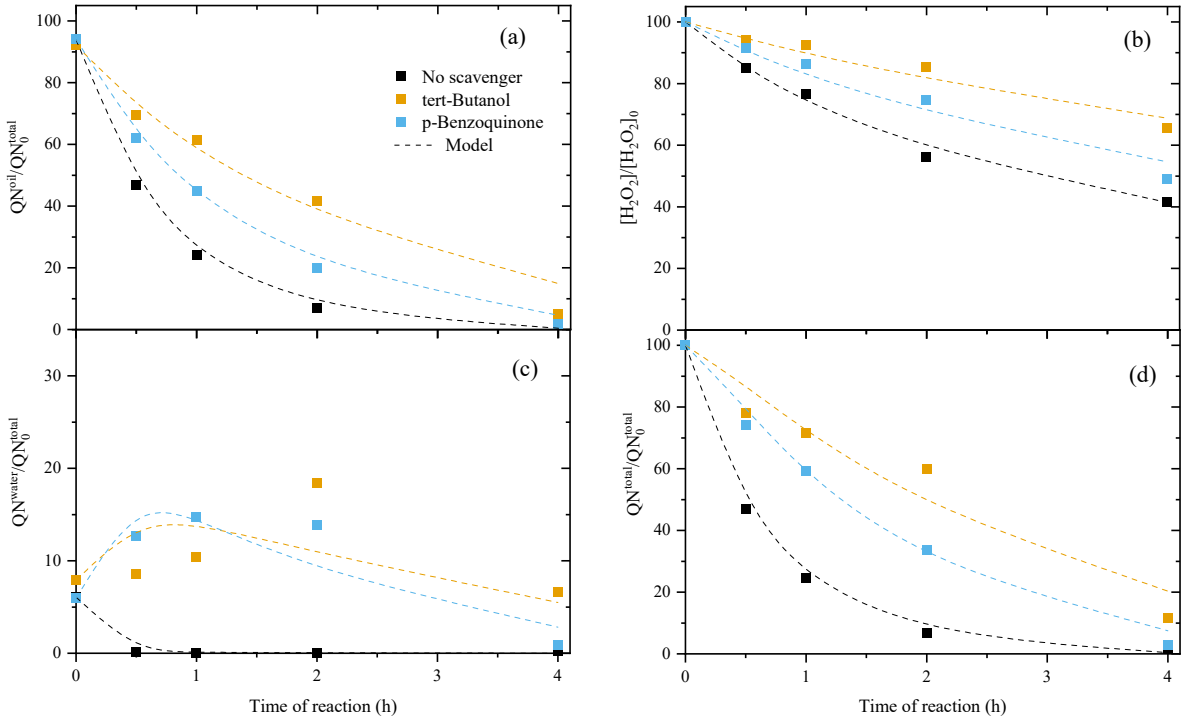

Fig.1. (a) QN removal from fuel, (b) H_2O_2, (c) QN in aqueous phase and (d) overall QN abatement. Conditions: $[QN]_0$ = 500 mg L^{-1} in 2,2,4-trimethylpentane, $[H_2O_2]_0$ = 12 g L^{-1}, O/W volume ratio = 80:20, T = 70 °C, [POL-OX@NiFe] = 2.5 g L^{-1}, pH_0 = 3.0. Dashed lines represent the kinetic model described elsewhere[3]

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO (DOI: 10.54499/UIDB/00690/2020 and 10.54499/UIDP/00690/2020) and SusTEC (DOI: 10.54499/LA/P/0007/2020); and by *Sociedade Ponto Verde* with the project "*Estudo técnico-económico para a valorização de resíduos de embalagens plásticas na produção de nanotubos de carbono*".

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EES - D3 - P34
Removal of bisphenol-A by catalytic wet peroxide oxidation using sustainable carbon nanotubes

Thoriso Kotsoane[1], Adriano Silva[1], Helder T. Gomes[1], Fernanda F. Roman[1]
[1]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal

Typical wastewater plants fail to remove compounds found in the ng/L - µg/L range[1], resulting in a pressing need to develop low-cost solutions for the removal of human-use substances (HUS)[1]. In this context, catalytic wet peroxide oxidation (CWPO) is a hydroxyl radical-based technology that can eliminate a wide range of HUS at mild operating conditions given that active catalysts are used[2]. Another current issue is the generation and accumulation of plastic solid waste (PSW), which can be upcycled into carbon nanotubes (CNTs), thus substituting fossil-derived precursors in the obtention of advanced materials[3]. In this work, a CNT was synthesized from PSW provided by the local waste management company. More details about synthesis conditions can be found here[3]. The CNT was used as catalyst on the CWPO of bisphenol-A (BPA) as a microplastic representative. The waste-derived CNT demonstrated high catalytic activity, which when compared to the non-catalytic run (NC) resulted in a 2.5× and 63× increase in BPA removal and H_2O_2 consumption, respectively, at 2 h of reaction. High TOC removals and efficiency of H_2O_2 consumption ($\eta_{H_2O_2}$) were achieved in the presence of the CNT, as shown in Figure 1.

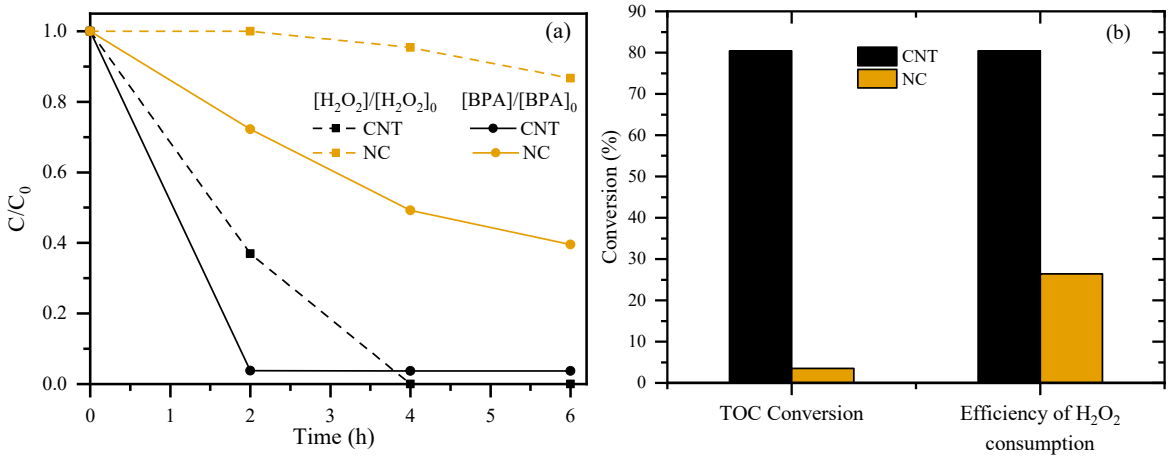

Fig.1. (a) CWPO of BPA and (b) TOC conversion and $\eta_{H_2O_2}$. Conditions: $[BPA]_0$ = 100 ppm, $[H_2O_2]_0$ = 536 ppm, pH_0 = 3.5, T = 80 °C, C_{cat} = 2.5 g L^{-1}. NC in the absence of hydrogen peroxide.

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO (DOI: 10.54499/UIDB/00690/2020 and 10.54499/UIDP/00690/2020) and SusTEC (DOI: 10.54499/LA/P/0007/2020); and by *Sociedade Ponto Verde* with the project "*Estudo técnico-económico para a valorização de resíduos de embalagens plásticas na produção de nanotubos de carbono*".

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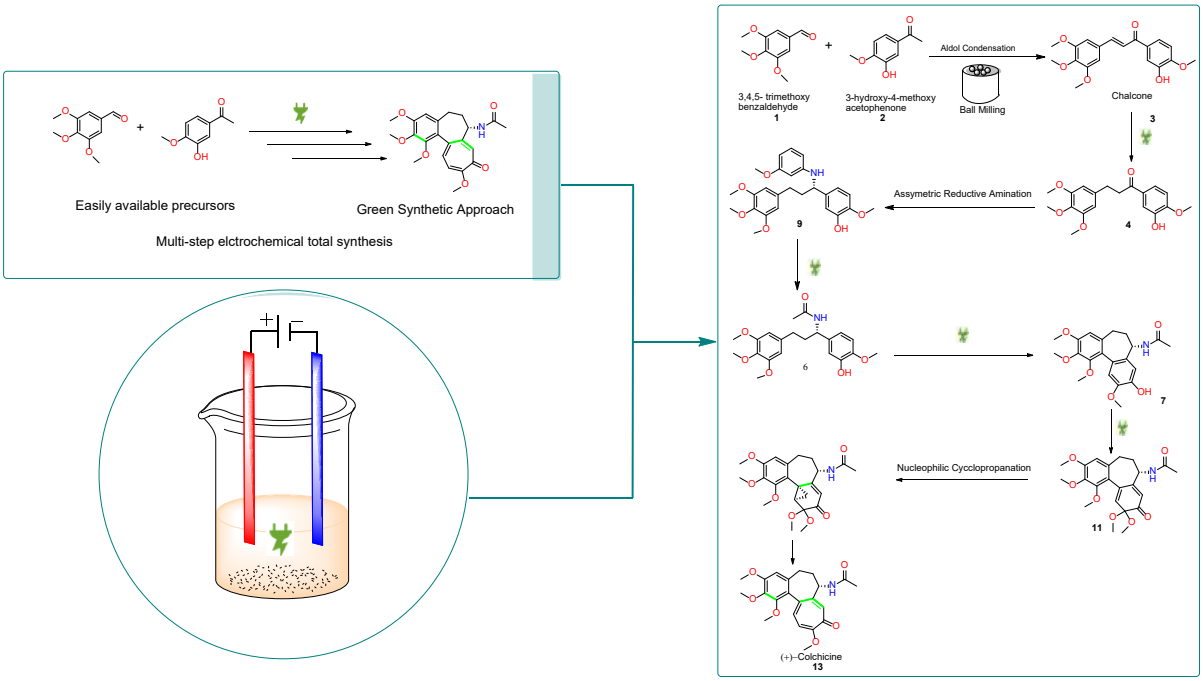
EES - D3 - P35
Electrochemical approach towards the total synthesis of (-)-colchicine

Syed Muhammad Shakib Kazmi
Loughborough University, UK

Colchicine is a pharmaceutically important alkaloid whose total synthesis remains challenging due to its structural intricacy and stereochemical complexity. In this study, we report a sustainable electrochemical strategy for the synthesis of (-)-colchicine, aiming to replace hazardous reagents while improving overall process efficiency. In the asymmetric synthetic pathway, four of the eight steps were performed electrochemically, including electrochemical reduction, intramolecular cyclisation, deprotection, and dearomatisation reactions. In addition, the synthetic route incorporates a solvent-free mechanochemical transformation and an asymmetric reductive amination step to introduce enantiopurity. Collectively, these methodologies provide a more sustainable and environmentally benign approach to the total synthesis of colchicine. The electrochemical transformations proceeded in moderate to high yields, demonstrating the potential of electrochemical techniques to enhance yield, selectivity, and operational safety. This work highlights the promise of electrochemical synthesis as a green and efficient platform for constructing complex natural products.



EES - D3 - P36

Nano-calcium driven degradation of dichlorodiphenyltrichloroethane in soil: Efficiency assessment and underlying mechanisms

Bienvenu Kwizera[1], Kato Nanami[1], Mitoma Yoshiharu[1]

[1]Chuo University, Graduate School of Science and Engineering, Dept. of Civil, Human and Environmental Science and Engineering, Mitoma Laboratory (Environmental energy laboratory), Japan

Dichlorodiphenyltrichloroethane (DDT) introduced in the 1940s as an effective insecticide, has since become recognized as a globally persistent organic pollutant. Its chemical stability, strong adsorption to soils, and ability to bioaccumulate allow DDT and its metabolites particularly DDE and DDD to persist in ecosystems for decades. Despite widespread regulatory restrictions and bans, DDT residues remain detectable worldwide, highlighting the need for effective remediation strategies.

This study evaluated the degradation of DDT in low-moisture Akadama sandy soil (5.1% moisture),(a granular volcanic soil widely used in Japan), artificially contaminated with 100 mg of DDT per 100 g of soil. Using a ceramic grinding mortar equipped with a rotary stirring system (40 rpm), 5 g subsamples of the spiked soil were treated with nano-calcium (nCa) at dosages of 0.5 g and 5 g for 1 h and 24 h under both air and nitrogen atmospheres. Post-treatment, DDT leaching tests were conducted using 50 mL of toluene for extraction, followed by quantification via GC-MS.

Results demonstrated that the highest degradation efficiency of 92% was achieved under aerobic conditions with 5 g nCa, compared to 75% under nitrogen. The lower dosage of 0.5 g nCa resulted in similar efficiencies 64% across both atmospheric conditions. Depending on each country: WHO guideline threshold of 1 g/m². nCa dosage emerged as the dominant factor influencing degradation, whereas stirring time showed minimal effect under aerobic conditions and only slight improvement under nitrogen. Overall, nCa exhibited strong potential as a soil remediation agent for DDT-contaminated environments. Further studies are recommended to optimize treatment parameters and elucidate the dechlorination pathways driving nCa-mediated DDT breakdown.

Acknowledgements: This research was supported by the SICORP program of the Japan Science and Technology Agency (JST) under the Africa–Japan Collaborative Research (A-J CORE) initiative. It was conducted as part of the project “Sustainability Challenge in Africa: Purification of Contaminated Soil Using Nano-Calcium and Its Recycling into Eco-Fertilizer and High-Strength Concrete (SCA-CEFC).

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EES - D3 - P37

Non-stoichiometric CuAgSe doped with Zn or Fe: Mechanochemical synthesis and thermoelectric properties

Dáša Drenčaková[1,2], Marcela Achimovičová[1], Emmanuel Guilmeau[3], Jaroslav Briančin[1], Viktor Puchý[4]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia; [2]FMMR, Technical University of Košice, Slovakia; [3]CRISMAT, CNRS, Normandie University, France; [4]Institute of Materials Research, Slovak Academy of Sciences, Slovakia

Thermoelectric materials can convert heat to electricity and vice versa, offering a potential way to utilize waste heat. Among functional thermoelectric materials are also metal chalcogenides, including ternary CuAgSe. The application of environmentally friendly synthetic methods is an increasingly important factor in chemistry nowadays. Ball milling offers a simple, one-pot, solvent-free, time-saving method at room temperature and ambient pressure.

This study was performed in order to investigate the influence of doping by various amounts of zinc or iron on the thermoelectric properties of non-stoichiometric $Cu_{2-x}Ag_xSe$. Previously published works differ in (non-)stoichiometry of CuAgSe, in selected dopant, and in synthesis method, but similarly show significant changes in thermoelectric properties of doped CuAgSe.[1,2]

Mechanochemical syntheses of $Cu_{0.6}Ag_{1.4}Se$ doped with 3, 6, 10% of Zn or Fe over Cu were carried out in a planetary ball mill Pulverisette 6 (Fritsch, Germany) from elemental powders. Syntheses were completed after only 7 min of milling, which was confirmed by XRD analysis. For the consolidation of the prepared powders into pellets, the SPS method was used. The phase composition, morphology, specific surface area, mean particle size, and thermoelectric properties of the samples have been studied.

Acknowledgement: This work was supported by the Slovak Grant Agency VEGA (project 02/0036/23) and the Slovak Research and Development Agency (contract no. APVV-24-0353).

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EES - D3 - P38

Magnetic heating-assisted methanol synthesis from CO_2 and H_2 for Power-to-X applications

Anej Blažič[1,2], Anja Sedminek[3], Stanislav S. Yakushkin[1], Blaž Likozar[1], Janvit Teržan[1]

[1]National Institute of Chemistry, Slovenia; [2]University of Nova Gorica, Slovenia; [3]Institute "Jožef Stefan", Slovenia

Methanol is the simplest aliphatic alcohol and is widely used as a solvent, fuel, and energy storage medium. In addition to its traditional applications, methanol is receiving increasing attention in Power-to-X (PtX) technologies, which convert excess renewable energy into chemical energy. In this context, methanol can be produced from captured CO_2 and H_2 obtained via water electrolysis. Producing carbon-neutral fuels is not only beneficial for the environment but also enables more efficient energy storage and allows seamless integration into the existing fuel infrastructure. Thus, methanol is a promising energy carrier for the storage and transportation of renewable energy.[1-2]

In this study, methanol synthesis was carried out using magnetic heating, a process that relies on an alternating magnetic field (AMF) to induce localized and rapid heating in ferromagnetic nanoparticles. To achieve this, a magnetic nanocomposite consisting of CoFe nanoparticles and a silica-alumina shell was prepared. This magnetic support was used to prepare the methanol catalyst by coprecipitating copper and zinc onto the silica-alumina shell, yielding the final catalysts for methanol synthesis.

Fig. 6. Left: STEM image of CoFe nanoparticles within a silica-alumina shell. Middle: quartz reactor containing the catalyst. Right: induction coil placed around the reactor for magnetic heating.

Catalytic experiments were conducted in a fixed-bed induction reactor using 200 mg of catalyst and a constant gas flow of 50 mL/min (H_2: CO_2 = 3:1) at 30 bar and temperatures between 200 and 300°C. At 250°C, 0.5 mol% methanol was detected in the gas phase with very high selectivity. This can be attributed to the silica-alumina shell, which acts as a barrier and suppresses undesired side reactions, such as methanation and Fischer-Tropsch synthesis, of the magnetically heated CoFe cores. These results demonstrate the feasibility of methanol synthesis via magnetic heating and highlight its potential for PtX applications.

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EES - D3 - P39

Water-induced structural deactivation of zeolite-supported magnesium chloride and its effect on ammonia sorption stability

Aleksandra Zamljen[1,2], Anže Prašnikar[1], Alen Vizintin[1], Matej Huš[1], Blaž Likozar[1]
[1]National Institute of Chemistry, Slovenia; [2]Faculty of Chemistry and Chemical Technology, Slovenia

Ammonia is emerging as a carbon-neutral energy carrier, but its conventional production remains energy intensive[1]. Solid sorbents, especially metal halides, offer a promising alternative to conventional ammonia separation by condensation. Magnesium chloride is especially attractive for ammonia separation and storage applications due to its strong and reversible coordination with ammonia[2]. However, its practical application is still limited by structural instability and high sensitivity to moisture[3], motivating a deeper understanding of its degradation behaviour.

This study provides a mechanistic and quantitative assessment of moisture- and cycling-induced degradation of $MgCl_2$-impregnated ultra-stable Y (USY) zeolite[4]. Using FTIR and XPS analysis, it was found that water exposure progressively deactivates $MgCl_2$ active sites through the formation of oxygen-containing magnesium species, including MgO and MgOHCl. Pre-ammoniation of the material with ammonia and density functional theory calculations provide evidence that pre-adsorbed ammonia does not inhibit water absorption and demonstrate that ligand exchange reactions are thermodynamically favoured over molecular water intercalation, clarifying the degradation pathway. Temperature-programmed desorption measurements reveal that co-exposure to ammonia and water modifies the magnesium coordination environment, which weakens ammonia binding. Furthermore, ammonia cycling under dry conditions was also investigated. The results show that ammonia cycling causes irreversible structural changes through the formation of defect-rich crystalline regions that reduce ammonia capacity. Despite these degradation mechanisms, sorption experiments demonstrate that $MgCl_2$/USY maintains a measurable ammonia uptake at high-temperature (300 °C, 8 bar), indicating potential for use in integrated ammonia sorption-enhanced ammonia synthesis. These findings help establish operational limits for the practical application of supported magnesium chloride sorbents.

The work was funded by the European Union – Horizon Europe, Grant Agreement [101058643], HySTrAm: Hydrogen Storage and Transport using Ammonia, and by the Slovenian Research and Innovation Agency through core funding P2-0152, infrastructure funding I0-0039, and the research projects N2-0291 and TN-03. The research was (co-)funded under the HyBReED project, supported by the European Union – NextGenerationEU. Computational resources at the HPC system Vega at the Institute of Information Science, Maribor, Slovenia were provided by the HPC RIVR consortium and EuroHPC JU.

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EES - D3 - P40

Redox electrolyte-assisted hybrid energy storage with optimized cathode/anode ratio of cobalt hexacyanoferrate and activated carbon

Hye-Seon Park[1,2,3], Seung-Yeop Yoo[1,2,3], Sang-Eun Chun[1,2,3,*]

[1]School of Materials Science and Engineering, Kyungpook National University, Republic of Korea; [2]Innovative Semiconductor Education and Research Center for Future Mobility, Kyungpook National University, Republic of Korea; [3]Research Institute of Automotive Parts and Materials, Kyungpook National University, Republic of Korea

Hybrid energy storage devices combine a battery-type (faradaic) electrode with a capacitive-type electrode to simultaneously achieve high energy and power densities. However, mismatches in reaction kinetics and charge storage capacity can deteriorate both energy and power densities. Here, an open-framework cobalt hexacyanoferrate (CoHCF) cathode is introduced to enable rapid Na^+ insertion/extraction kinetics compatible with the capacitive-type electrode, thereby mitigating the kinetic mismatch in a hybrid energy storage system.

Activated carbon (AC) was employed as the anode, and heptyl viologen dibromide ($HVBr_2$) was used as the redox-active electrolyte. During charging, Na^+ ions deintercalate from the CoHCF cathode, while the anode accommodates Na^+ adsorption on activated carbon accompanied by the reduction of HV^{2+} species (Fig. 1). To resolve capacity mismatch, hybrid cells with different cathode-to-anode mass ratios were systematically designed and evaluated. As a result, the optimized CoHCF//AC hybrid cell with a cathode-to-anode mass ratio of 1:2 delivered a maximum power density of 516 W kg^{-1} and an energy density of 44 Wh kg^{-1}.

The $HVBr_2$ electrolyte contributes to anode-side charge storage through reversible redox reactions. Upon reduction, the resulting HV species ($HV^{\bullet+}$) adsorb on the anode surface to form a surface film that suppresses self-discharge, leading to a capacity retention of 78% after 72 h. Through rational material selection and device design, this work demonstrates a hybrid energy storage system that simultaneously overcomes kinetic and capacity mismatches between electrodes while delivering high energy and high power densities. The proposed hybrid device shows strong potential for applications requiring rapid charge–discharge operation combined with high energy storage capacity.

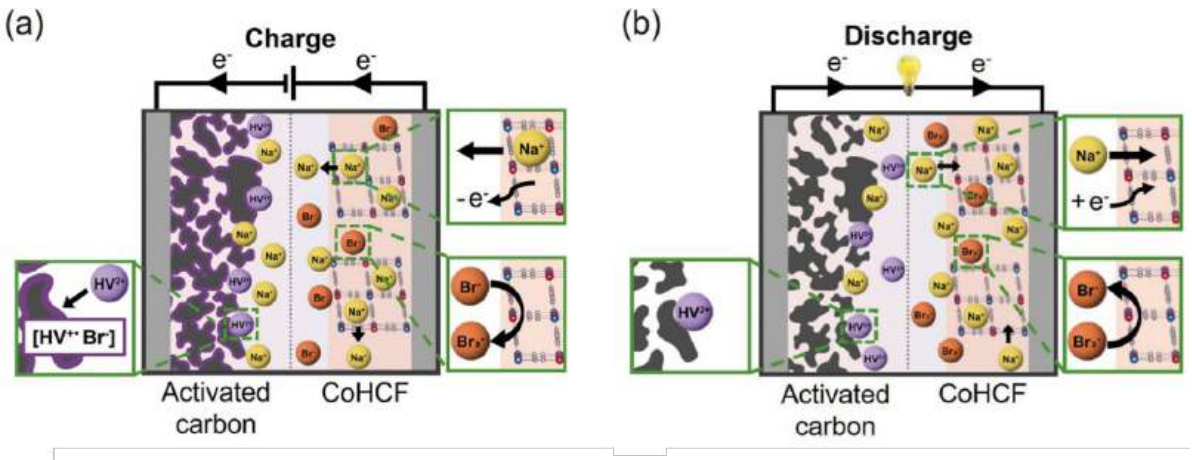

Fig. 1. Schematic illustration of the energy storage mechanisms in a hybrid energy storage device under (a) charged and (b) discharged states

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korean government(MIST) (No.2022R1A2C1009922)

EES - D3 - P41
Silk fibroin solid electrolyte membranes for sustainable sodium-ion batteries

Paula Barbosa[1], Beatriz Rocha[1], Filipe Rodrigues[1], Rita Veloso[2], Filipe Figueiredo[1]
[1]CICECO – Aveiro Institute of Materials, Dept. of Physics, University of Aveiro, Portugal; [2]Vasco da Gama CoLAB – Energy Storage, PORTIC, Portugal

The growing demand for sustainable and cost-effective energy storage technologies has intensified interest in sodium-ion batteries as an alternative to lithium-based systems, owing to the natural abundance and wide geographical distribution of sodium. However, the development of safe and efficient solid-state electrolytes remains a critical challenge for the practical implementation of sodium-ion batteries.
In this work, silk fibroin is explored as a bio-based polymer matrix for the development of solid electrolyte membranes tailored for sodium-ion battery applications. Silk fibroin is a renewable and biodegradable biopolymer that combines excellent film-forming ability, mechanical robustness, and structural tunability, making it particularly attractive for solid-state electrochemical devices. By incorporating sodium salts and selected plasticizing agents, flexible fibroin-based membranes with enhanced ionic transport properties are obtained.
The resulting solid electrolyte membranes exhibit ionic conductivities in the 2 $mS \cdot cm^{-1}$ range at ambient temperature and high humidity, together with good thermal stability and structural integrity. The relationship between fibroin molecular structure and ion transport is discussed, highlighting the role of polymer chain organization and amorphous domains in facilitating sodium-ion conduction. These results demonstrate that silk fibroin-based electrolytes are a promising sustainable platform for the development of safer and environmentally friendly solid-state sodium-ion batteries.

Fig. 1. Silk Fibroin as polymer electrolyte membrane.

Acknowledgements: This work was financed by the BioEESC project (COMPETE2030-FEDER-00779500) and within the scope of the project CICECO-Aveiro Institute of Materials, UID/50011 & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC), financed by national funds through the FCT/MCTES (PIDDAC). Acknowledgments are also due to FCT/MCTES for the P. Barbosa (2023.06523.CEECIND) contract.

EES - D3 - P42

High-temperature structural and microstructural evolution of Ni- and Mn-doped $LaCoO_3$ perovskites

Dora Balen[1], Martina Vrankić[1], Vendula Bednaříková[2], Jasminka Popović[1], Serhii Tkachenko[2], Michaela Remešová[2], Ladislav Čelko[2]

[1]Ruđer Bošković Institute, Croatia; [2]Central European Institute of Technology, Brno University of Technology, Czech Republic

$LaCoO_3$ perovskites are beneficial for photovoltaics, catalysis, and energy storage due to their chemical stability and resilience.[1,2] Cooperative rotations of oxygen octahedra give its crystal structure trigonal symmetry, derived from the ideal cubic perovskite ABX_3 (A = La^{3+}, B = Co^{3+}, X = O^{2-}). Transition metal doping at A- and/or B-sites enhances structural and electrical characteristics, revealing new functions.

We investigates the structural evolution of $LaCoO_3$, $LaCo_{1-x}Ni_xO_3$ (x = 1.3 at.%, 2.9 at.%), and $LaCo_{1-x}Mn_xO_3$ (x = 1.7 at.%, 2.8 at.%) at temperatures up to 1000 °C, focusing on cation distribution at various temperature intervals using laboratory X-ray diffraction during controlled heating and gradual cooling. In addition to assessing diffraction line broadening, we explain temperature-induced variations in the oxygen positional parameter, La–O and Co/Ni(Mn)–O distances, and Co/Ni(Mn)–O–Co/Ni(Mn) angles calculated from structural refinements. Field-emission scanning electron microscopy micrographs of samples before/after slow cooling show reveal the effect of thermal treatment. Diffraction patterns showed that all samples were nanocrystalline and retained the *R*-3*c* space group's hexagonal axes within the temperature range. Ni- and Mn-doped $LaCoO_3$ exhibited increased unit cell parameters and diffraction line broadening under ambient conditions; however, cation distribution did not change significantly with temperature. Heating $LaCoO_3$ and Ni- and Mn-doped $LaCoO_3$ perovskites to 1000°C, followed by cooling to ambient temperature, enhances the resolution of hexagonal structure-related doublet peaks in powder XRD patterns. At elevated temperatures, $LaCoO_3$ exhibits dynamic oxygen octahedral rotations resulting in a higher-symmetry pseudo-hexagonal arrangement that improves lattice coherence and crystallite ordering during cooling. Heating reduces microstrain, sharpening doublet reflection splitting and significantly alters oxygen positional features and metal-oxygen distances, which control this perovskite family's catalytic and electrical capabilities.

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EES - D3 - P43

Controlled autoxidation of heavy petroleum residues as a low-cost route to synthesize carbon nanotubes

Ajay Sharma[1], Muhammad N. Siddiquee*[1,2]

[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals,Saudi Arabia; [2]Dept. of Chemical Engineering, King Fahd University of Petroleum & Minerals, Saudi Arabia

Carbon nanotubes (CNTs) demand is growing globally at a CAGR of 13.6% due to their wide range of industrial applications, including reinforcement fillers in composites, conductive additives in batteries and supercapacitors, electromagnetic interference shielding materials, sensors, membranes, and catalyst supports. Conventional CNTs are commonly synthesized from methane or acetylene via chemical vapor deposition, arc discharge, or laser ablation, at a production cost of approximately $10–50 per gram. On the other hand, heavy petroleum residues provide a low-cost ($1 per kg), carbon-rich, and more environmentally friendly alternative. This study explores heavy oil residues derived asphaltenes as low-cost alternative precursors for CNTs synthesis. The residues were subjected to controlled autoxidation via air blowing without mixing at relatively low temperatures (≤280 °C) for varying durations. Following oxidation, asphaltenes were isolated using n-heptane as the precipitating solvent and subsequently employed as precursors for carbon nanotube synthesis via a template-assisted pyrolytic growth method. Controlled free-radical oxidation enhances precursor properties, including increased viscosity, reduced volatility, changes in elements and functional groups, changes in molecular weights and improved cross-linking, and higher softening point and aromaticity. The synthesized CNTs were characterized using SEM, XRD, and Raman spectroscopy analyses. During SEM analysis, CNTs exhibited an aligned CNT growth and bundled multi-walled CNTs with diameters ranging from ~50 to 200 nm. XRD confirmed the formation of partially graphitized, turbostratic multi-walled CNTs. From the relative intensities of the Raman G and D bands, the degree of graphitization of the produced CNTs were estimated as IG/ID ≈ 0.9–1.2, indicating improved graphitic ordering and reduced defect density upon oxidation pretreatment. These findings demonstrate a promising route for converting low-value petroleum residues into CNTs, supporting economic diversification of refinery by-products, while emphasizing the need for further optimization of graphitization and purity to enable large-scale, high-performance applications.

Keywords: Carbon nanotubes; Heavy vacuum gas oil; Precursors; Autoxidation (air blowing); Sustainable materials.

Acknowledgements: The author(s) wish to acknowledge the Interdisciplinary Research Center for Refining & Advanced Chemicals (IRC-RAC) at King Fahd University of Petroleum & Minerals (KFUPM) for sponsoring this research, under grant number INRC 2514.

EES - D3 - P44

Optimizing solvent roles in catalytic lignin liquefaction: Efficient pathways to phenolic monomers and bio-oil

Wajahat Waheed Kazmi[1], Faysal M. Al-Khulaifi[1]

[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Saudi Arabia

Lignin, one of the three major components of lignocellulosic biomass, is generated as a byproduct of pulping and bioethanol industries, with an estimated annual production of about seven million tons. Despite its abundance, lignin remains largely underutilized, yet it represents a promising renewable feedstock for the production of biofuels, phenolic monomers, and other value-added chemicals. Among emerging conversion pathways, liquefaction has gained attention as an effective route for transforming technical lignins, such as Kraft lignin, into high-quality liquid products. In this study, the effects of key liquefaction parameters, including temperature, reaction time, and solvent type, on lignin depolymerization were systematically investigated under supercritical conditions. Product yield, composition, and quality were evaluated using GC-RGA, GC-SIM-DIS, GC–MS, thermogravimetric analysis, and elemental analyses. Catalytic upgrading was performed using a Ni-based catalyst in supercritical alcohols without the use of an external hydrogen source, enabling a more sustainable upgrading strategy. The use of supercritical alcohols facilitated simultaneous depolymerization, esterification, hydrogenation, decarbonylation, and decarboxylation reactions, resulting in a significant reduction in oxygen content and an increase in the higher heating value of the produced bio-oils. Particular emphasis was placed on maximizing the yield of phenolic monomers, which are important intermediates for fuels and chemical synthesis. Short-chain alcohols (C_1–C_3) served as both solvents and hydrogen donors, promoting in situ hydrogen generation and suppressing char formation. Under optimized reaction conditions, solvent consumption was substantially reduced while maintaining high product selectivity and stability. Catalyst performance and structural stability were examined using transmission electron microscopy, N_2 physisorption, and X-ray diffraction. The upgraded oils were further analyzed to determine phenolic monomer distribution, overall yield, and energy content. The results demonstrate that supercritical alcohols provide an efficient and sustainable medium for lignin depolymerization, offering mechanistic insight into solvent–lignin interactions and a viable pathway for lignin valorization toward renewable fuels and chemicals.

Acknowledgements: The authors acknowledge the support provided by the Interdisciplinary Research Center for Refining and Advanced Chemicals (IRC-RAC) at King Fahd University of Petroleum and Minerals (KFUPM), under project # INRC2539.

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EES - D3 - P45
Solvent-free upcycling of plastic waste to aromatics with multi-shelled hollow sphere

Muhammad Waqas[1], Muhammad Naseem Akhtar[1,2*]
[1]*Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of* Petroleum & Minerals*, Saudi Arabia;* [2]*Dept. of Chemistry, King Fahd University of Petroleum & Minerals, Saudi Arabia*

Typically, a metal oxide-zeolites catalyst is usually produced either by physically mixing metal oxide nanoparticles as dopants with the zeolite substrate, or by an impregnation process, resulting in an architecture, where metal oxide nanoparticles are dispersed randomly on the zeolite.[1] As a result, the uneven distribution of metal oxides on zeolites catalyzed the conversions instantly rather than sequentially. Furthermore, the metal oxides and zeolites components typically catalyze the initial and subsequent reactions in the tandem catalysis process to yield aromatics and the products created in the first stage on the metal oxide site may diffuse out without undergoing further reactions on the zeolite phase. Therefore, a random architecture is not optimal for achieving the highest efficiency and desired sequence in the tandem reaction. In addition, aromatization requires adequate acid sites (both Brønsted and Lewis) and shape-selective microporous structures to facilitate the complex reaction cascade (cracking, oligomerization, cyclization, dehydrogenation). We propose a generally applicable and simple synthesis method for facet-controlled nanocrystals@metal oxides@zeolites multi-shelled hollow spheres with predetermined metal-zeolite spatial organization and short diffusion length as illustrated in Figure 1. The developed preparation method allows control over different structural parameters and chemical compositions. The step-by-step conversion from the precursor material to the final solid catalyst will be monitored and the essential mechanisms for the involved self-assembly and hollowing behaviors will be revealed. We believe that the proposed synthesis has numerous advantageous and has potential to outperforms the conventionally synthesized materials via precipitation and impregnation procedures in the selective production of aromatics by upcycling of plastic waste. We will demonstrate that each structural engineering element in nanocrystals@metal oxides@zeolites multi-shelled hollow spheres, including the hollow-sphere design, core-shell spatial organization and “cage” effect of the H-ZSM-5 shell, contributes to the improvement of catalytic performance.

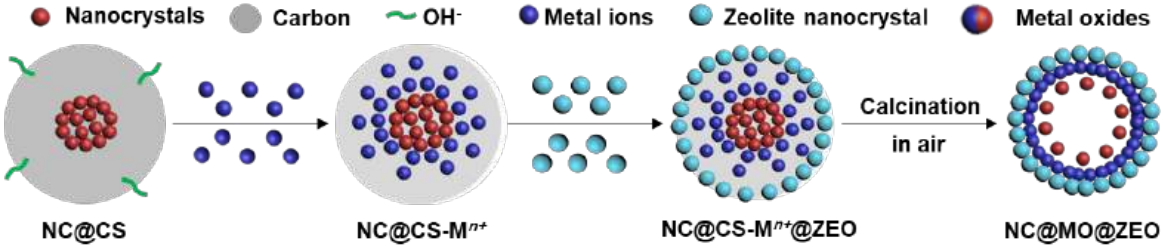

Fig. 1. Schematic illustration of the synthesis of nancrystals@metaloxides@zeolites hollow spheres

Acknowledgements: The authors acknowledge the support of King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia.

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EES - D3 - P46
Shrimp shell waste as a green resource for rare earth element recovery

Nicole Ferreira[1,2], Thainara Viana[1], Cláudia Nunes[3], Bruno Henriques[1], Eduarda Pereira[1]
[1]LAQV-REQUIMTE – Associated Laboratory for Green Chemistry, Dept. of Chemistry, University of Aveiro, Aveiro, Portugal; [2]CICECO, Dept. of Chemistry, University of Aveiro, Aveiro, Portugal; [3]CICECO, Dept. of Materials and Ceramics Engineering, University of Aveiro, Aveiro, Portugal

The growing demand for rare earth elements (REEs), driven by their essential role in clean energy technologies such as wind turbines and electric vehicles, raises critical supply, environmental, and geopolitical concerns[1]. NdFeB permanent magnets, containing REEs such as Nd, Pr, Dy, and Gd, generate significant waste both during manufacturing (15–30%) and at end-of-life (EoL)[2,3], highlighting the need for sustainable recovery strategies aligned with circular economy principles.
This study investigates shrimp shells (SS), an abundant and low-cost seafood-processing biowaste, as a natural biosorbent for the selective recovery of REEs from multi-element solutions simulating leachates of EoL NdFeB wind turbine magnets. Batch sorption experiments were conducted under varying pH, salinity, ion concentration, and sorbent dosage using synthetic solutions containing B, Ni, Co, Nd, Dy, Pr, and Gd at 100 µM.
Untreated shrimp shells outperformed thermally treated materials (400–600 °C), achieving >98–99% REEs removal while limiting the co-removal of competing metals such as Co (≈28%), Ni (≈27%), and B. Response surface methodology identified sorbent dosage and initial ion concentration as the most influential parameters, with optimal REEs selectivity at pH 3.0 and no significant effect of salinity. Under optimised conditions, 80–85% of REEs were selectively removed from simulated magnet leachates.
Kinetic studies showed rapid adsorption, reaching equilibrium within 6 h, with the Elovich model providing the best fit. Equilibrium data followed the SIPS isotherm, yielding maximum adsorption capacities of 75.5–89.7 mg/g. Desorption experiments demonstrated that dilute nitric acid (0.1 M) enabled >85% recovery of adsorbed REEs.
Overall, this work highlights raw shrimp shell waste as an efficient, selective, and sustainable biosorbent for REEs recovery from complex secondary resources.

Acknowledgement: This work received financial support from PT national funds (FCT/MCTES, Fundação para a Ciência e Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) through the REQUIMTE (UID/50006 – Laboratório Associado para a Química Verde – Tecnologias e Processos Limpos) and CICECO-Aveiro Institute of Materials (UIDB/50011/2020 & UIDP/50011/2020). This work is funded by COMPETE2030-FEDER-00847800. Nicole Ferreira thanks the Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior for their PhD grant ref. 2022.13017.BD. Thainara Viana thanks the Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior for their PhD grant ref. 2022.13015.BD.

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EES - D3 - P47

Synthesis and catalytic evaluation of $NiO–Al_2O_3$ catalyst for steam methane reforming

Ghulam Asghar[1], Safyan Akram Khan[2,*]

[1]IInterdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum and Minerals, Saudi Arabia

Hydrogen serves as a crucial energy carrier in the shift to low-carbon and sustainable energy systems, with uses in clean power generation, chemical processing, and fuel cell technology. Steam methane reforming (SMR) remains the most important industrial method for hydrogen production; however, developing efficient, stable, and cost-effective catalysts is vital to enhance process performance and hydrogen output. In this study, a $NiO–Al_2O_3$ catalyst was created using a controlled chemical process and thoroughly characterized to evaluate its suitability for SMR.

The synthesized catalyst was characterized using X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, scanning electron microscopy (SEM), and temperature-programmed techniques to elucidate phase composition, surface properties, and metal–support interactions. Catalytic performance was evaluated in a fixed-bed reactor under steam methane reforming conditions. The $NiO–Al_2O_3$ catalyst demonstrated excellent activity, achieving 99 % methane conversion with a high hydrogen yield under the investigated operating conditions.

The enhanced performance is attributed to the high dispersion of NiO species on the Al_2O_3 support, strong metal–support interactions, and favorable surface characteristics that promote efficient methane activation. A clear correlation between synthesis, structural features, and catalytic performance is established. These results highlight the potential of $NiO–Al_2O_3$ as an effective catalyst for hydrogen production via steam methane reforming.

Acknowledgements: The authors gratefully acknowledge the financial support from King Fahd University of Petroleum and Minerals (KFUPM), Kingdom of Saudi Arabia, for supporting this research project.

EES - D3 - P48

Synthesis and evaluation of porous organic polymers for CO_2 capture

Aqeel Ahmad[1], Othman Charles S Al Hamouz[1,2]

[1]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Kingdom of Saudi Arabia; [2]Dept. of Chemistry, King Fahd University of Petroleum and Minerals (KFUPM), Kingdom of Saudi Arabia

The burning of fossil fuels has been a continuous contributor to atmospheric levels of carbon dioxide (CO_2) since the industrial revolution. In 2023, it reached a new peak of 425 parts per million (ppm), and this trend is only going to become worse in the coming decades. Potential candidates for minimizing the environmental effects of CO_2 emissions are porous polymer polymers (POPs), which are recognized for their exceptional stability and well-developed porosity. In this research, two newly synthesized POPs named PP7 and PP8 are prepared using triptycene and tetra-2-pyridinylpyrazine via Friedel-Crafts alkylation with and without dimethoxymethane, respectively. To confirm the synthesis, NMR, FTIR and XRD studies were conducted, and it was also noted that the polymers are thermally stable up to 300 ºC. The BET surface was also determined, and the values are 1027 and 699 m^2/g as shown in Figure 1a. The CO_2, CH_4, N_2 and H_2 gas adsorption studies were performed at 273 K and 298 K and PP7 performed well at both temperatures for all gases. Specifically, the CO_2 uptake values were 2.62 and 2.18 mmol/g (Figure 1b) and H_2 values are 5.10 and 4.59 mmol/g for PP7 and PP8 at 273K, respectively. The isosteric heat of adsorption (Q_{st}) was calculated using Clausius-Clapeyron equation and the results provided the higher values for CO_2 as compared to CH_4 and N_2 for PP7 and PP8. Based on these results, it can be elucidated that the prepared polymers are the potential materials for CO_2 capture and clean energy applications.

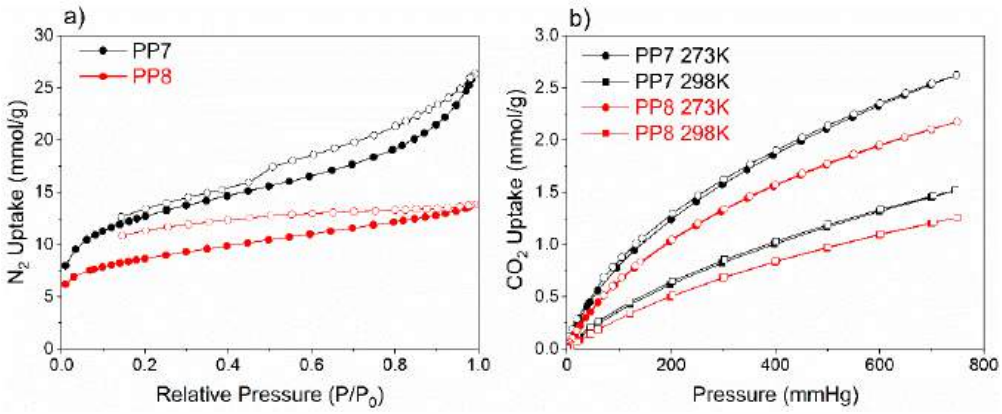

Fig. 1. PP7 and PP8 data of a) N_2 adsorption and desorption at 77K for surface area b) CO_2 adsorption data at 273K and 298K

Keywords: Polymerization, porous organic polymers, CO_2 capture, adsorption isotherms, environmental applications.

Acknowledgements: The authors are thankful to KFUPM university for providing the facilities to accomplish the research activities.

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EES - D3 - P50

Assessment of some organochlorine pesticides and toxic heavy metals in the road dust from a metropolitan city in Nigeria: Akure as a case study

Akinyinka Akinnusotu*[1,4], Benjamin, O. Opawale[2], [3]Eniayo, A. Komolafe

[1]Dept. of Science Laboratory Technology, University of Medical Sciences, Ondo City, Nigeria; *[2]Dept. of Science Laboratory Technology, Rufus Giwa Polytechnic, Owo, Nigeria*; *[3]Dept. of Food Science and Technology, Rufus Giwa Polytechnic, Owo, Nigeria*; *[4]Institute Environment and Human Health (TIEHH), Texas Tech University (TTU), Lubbock, Texas, USA*

Environmental pollutants are on the rise due to several anthropogenic activities in cities across the globe. Organochlorine (OC) pesticides are one of such pollutants used for various purposes. Heavy metals on the other hand have been reported for their numerous toxicities. Samples were taken from seven different locations and analysed using standard methods. The following OC pesticides congeners - α-HCH, β-HCH, γ-HCH (Lindane), and δ-HCH, popularly called the hexachlorocyclohexane were analysed. They are in the following range: BDL – 2.272 µg/kg for α-HCH, BDL – 10.080 µg/kg for β-HCH, 4.872 – 31.834 µg/kg for γ-Lindane, and BDL for δ-HCH. Lindane was detected from all the sampling locations with significant concentrations. The highest is from the sampling location 7 (SL 7) while the least is from the sampling location 5 (SL 5). The highest ∑ HCHs is from the sampling location 7 (SL 7) (41.914 µg/kg) while the least is from the sampling location 3 (SL 3) (7.146 µg/kg). The order of increase of the HCHs with the locations is SL 7 > SL 3 > SL 2 > SL 4 > SL 6 > SL 5 > SL 1. Source identification showed fresh, industrial and historical usage from some of the sampling locations. The concentrations of the selected toxic heavy (THM) metals are in the following range (mg/kg): Pb (0.49±0.00-0.72±0.00), Cd (0.15±0.00 - 0.32±0.00), As (0.06±0.01 - 0.37±0.00), Cu (1.35±0.00 – 3.24±0.00), Cr (1.70±0.00 - 3.58±0.00), Co (0.05±0.01 - 0.22±0.01), and Ni (0.43±0.05 - 0.92±0.00). The degree of their concentrations in the order of Co > As > Cd > Pb > Ni > Cu > Cr. The sources of heavy metals are similar with Pb having a different source. Lindane is predominant in road dust samples which can cause several environmental and human health problems including the THMs.

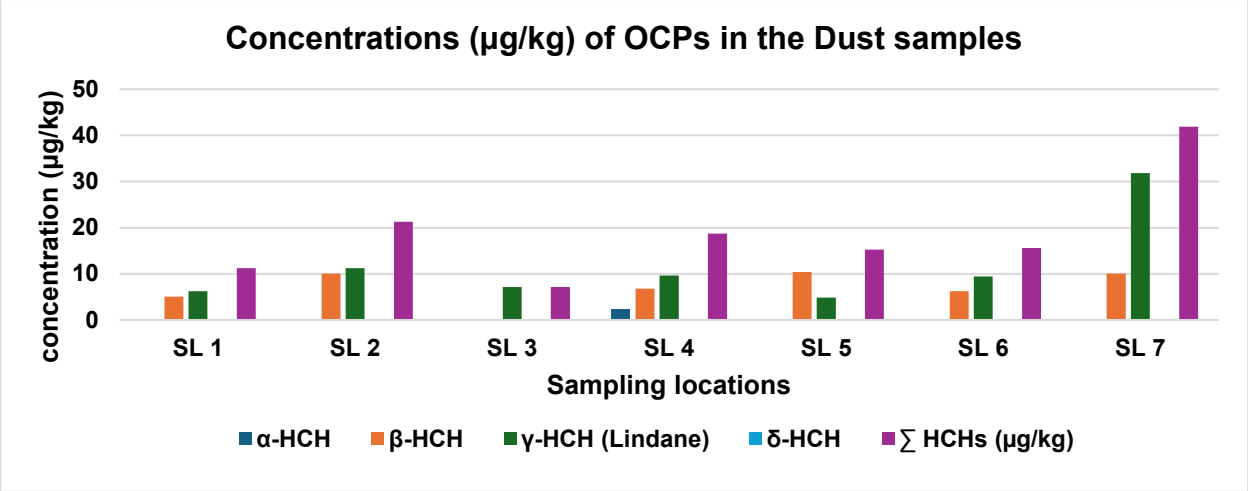

Fig.1. OCPs concentration (µg/kg) in the road dust samples from the locations

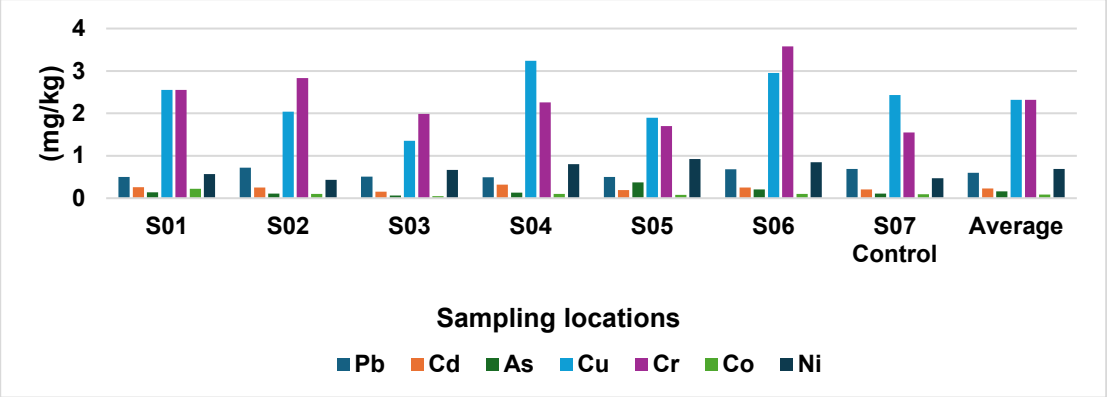

Fig. 2. Chart showing heavy metal concentrations across all the sampling locations

Key words: Toxic heavy metals, pesticides, HCHs, Road Dust, Lindane, health assessment.

Acknowledgement: The Tertiary Education Trust Fund (TETFUND) (TETF/DR&D/CE/POLY/OWO/IBR/2023/VOL III). TETFund conference intervention through University of Medical Sciences, Ondo-City, Nigeria. Special thanks to Prof. Todd Anderson and Dr. Seenivasan Subbiah of the Institute Environment and Human Health (TIEHH) Texas Tech University (TTU), Texas, USA. The effort of Dr. Francis Olawale Abulude of Science and Education Development Institute, Akure, Nigeria is appreciated.

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EES - D3 - P60

Removal of nitrogenous heteroaromatic compounds from gasoline using the deep eutectic solvent diethanolamine: glycerol

Omar Berkane[1], Hocine Sifaoui[1,*], Fabrice Mutelet[2], Hakim Belkhalfa[3]
[1]Bejaia University, Algeria; [2]Lorraine University, France; [3]Technical platform for physical and chemical analysis, Algeria

Among the gases that harm the environment and aquatic ecosystems are nitrogen oxides (NO_X), which are partly responsible for the greenhouse effect and acid rain. Their sources are numerous, but the primary source is the combustion of nitrogen compounds contained in hydrocarbons using in industry, transportation and domestic heating. These compounds end up in fuels (gasoline, diesel, kerosene, and heavy fuel oil) used in everyday human life. In recent years, a family of deep eutectic solvents (DESs) has been emerged. Thanks to their environmentally friendly properties, these solvents are classified as green solvents. These solvents are formed by mixing a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), resulting in a liquid phase with a melting point lower than that of its components in their pure state[1]. In this work, the DES, Diethanolamine: glycerol [1:2], was prepared and used to remove pyridine and quinoline from n-heptane, using the liquid-liquid extraction technical. N-heptane is considered as a model molecule for gasoline. To this end, two liquid-liquid equilibrium (LLE) systems {n-heptane + pyridine/quinoline + DES} were experimentally measured at 298.15 K and 1 atm. The obtained results are show in Fig. 1, the two ternary diagrams are category I type according to the classification of Sorensen et al.[2], with partial miscibility between n-heptane and DES and complete miscibility between the nitrogen compounds with n-heptane and DES. The experimental LLE values were correlated using the NRTL method[3] and the COSMO-RS model[4]. The NRTL correlation results are in very good agreement with the experimental values for two systems. In contrast, the COSMO-RS model results, while qualitatively consistent with the experimental results, show a more or less significant quantitative discrepancy between the two mixtures. In conclusion, the DES (Diethanolamine: glycerol) can be considered as a promising extracting agent for nitrogen compounds from gasoline.

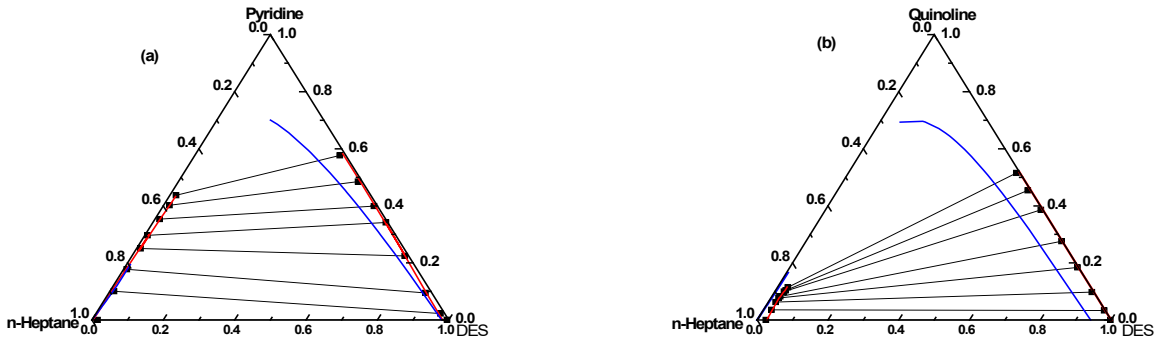

Fig. 1. Ternary LLE diagrams in molar fractions for systems: (a) (n-heptane + pyridine + DES), (b) (n-heptane + quinoline + DES), (–■–) Experimental measured tie lines; (–), NRTL binodal curve calculated; (–), COSMO-RS binodal curve calculated.

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EES - D4 - P01
Treatment of poly(vinyl chloride) and study of its pyrolysis outcomes

Emilia M. Kazek, Prof. James A. Sullivan
University College Dublin, Ireland

Pyrolysis is a chemical recycling method used for plastic waste management, which involves heating plastic waste to temperatures of 300-800˚C in the absence of oxygen to generate useful condensable and non-condensable products.
Poly(vinyl chloride) (PVC) is the third most widely produced plastic in the world, however progress in the pyrolysis of PVC has been hindered by the fact that it contains chlorine. The HCl generated from pyrolysis causes corrosion, slag formation, and the generation of toxic organochlorines.[1] In this work, the optimal conditions for PVC pyrolysis were determined using thermogravimetric analysis.
To combat the issues with chlorine and HCl in waste PVC, different PVC pre-treatment strategies for chlorine removal were studied. Thermal dechlorination was performed by low temperature pyrolysis in a thermogravimetric analyser. Solvothermal and non-thermal plasma treatments, which introduce oxygen species that partake in elimination and substitution reactions, were also investigated. The outcomes from PVC treated in these ways were compared with those from virgin PVC using thermogravimetric analysis and within a lab-scale pyrolysis reactor.
Heterogenous aluminosilicate catalysts have been shown to increase the rate of plastic degradation during pyrolysis, facilitating complete degradation at lower temperatures than in the absence of a catalyst.[2] The effects of aluminosilicate solid catalysts on the degradation of virgin and treated PVC were studied.

This project has received funding from the European Union HORIZON TMA MSCA Staff Exchanges (HORIZON-MSCA-2021-SE-01), grant agreement no. 101086071, project name “CUPOLA — Carbon-neutral pathways of recycling marine plastic waste”.

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EES - D4 - P02

High performance steam methane reforming via tuned metal support interactions in NiMg-Yb_2O_3 sesquioxide: Activity, stability, and coke resistance

Safyan Akram Khan, Muhammad Mansha[1], Shahid Ali[1], Ghulam Asghar[1], Sumaira Manzoor[1,*]
[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum and Minerals, Saudi Arabia

Recently, high-performance and coke-resistant catalysts are essential to produce hydrogen via steam methane reforming (SMR) at lower operating temperatures. In present work, NiMg-Yb_2O_3 catalyst with selective interactions between metals on the support is achieved through a controlled coprecipitation approach using ethylene glycol as a structure-directing medium, which produced a unique cauliflower-like morphology with high surface energy nanoparticles. The addition of Mg and Ni in Yb_2O_3 was effective in altering the physicochemical characteristics of the Yb_2O_3 base which promoted the dispersal of metals and the strength of interactions between metals and the support. The catalyst shows an excellent SMR activity with an excellent methane conversion of 97% and hydrogen production value of 92.75% at a low operating temperature of 650 °C. Cauliflower-like morphology enabled the enhanced diffusion of the reactants and exposure of the active sites, which led to high catalytic activity. Moreover, co-interaction of Ni, Mg and Yb_2O_3 greatly inhibited carbon deposition resulting in high stability and coke resistance in a long-term reaction time. These findings indicate that the resultant material fabricated via ethylene glycol-assisted coprecipitation of NiMg-Yb_2O_3 can attain morphology control to form effective low-temperature, high-efficiency SMR catalysts for hydrogen production.

EES - D4 - P03
Phase stability and thermodynamic properties of magnesium carbonates in salt solutions

Hagen Fiebig, Daniela Feyer, Gero Frisch
TU Bergakademie Freiberg - Institute of Inorganic Chemistry, Germany

The long-term safety assessment of radioactive waste repositories is largely based on thermodynamic modelling, which requires a robust understanding of chemical equilibria between host rock components, saline pore fluids, waste inventories, and engineered barrier materials. In particular, carbonate concentration and pH significantly impact the actinide solubility. In current rock-salt-based repository concepts, these parameters are planned to be actively controlled by the addition of MgO or $Mg(OH)_2$ respectively, which bind CO_2, ensure an alkaline pH of brines, and promote carbonate formation. So far however, the stability and transformation behavior of magnesium carbonate phases under repository-relevant ionic strengths remain insufficiently understood.
Current studies are thus focused on the exploration of any chemical equilibria involved in the system Mg^{2+}–Cl^-–OH^-–CO_2–H_2O, aiming to expand the Thermodynamic Reference Database (THEREDA).[1,2] The solid magnesium carbonate phases magnesite ($MgCO_3$), nesquehonite ($MgCO_3 \cdot 3\ H_2O$), hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4\ H_2O$), dypingite ($Mg_5(CO_3)_4(OH)_2 \cdot 5+x\ H_2O$), and chlorartinite ($Mg_2(CO_3)Cl(OH) \cdot x\ H_2O$) have been deemed most relevant, and syntheses have been established that reproducibly lead to well-defined solids as characterizations using P-XRD, SEM (e.g. Fig. 1), Raman, and TG-DSC have shown. The presented experimental setups designed to quickly establish equilibria with $MgCl_2$ solutions of differing concentrations at a given temperature and subsequently allowing for quantifying the composition of both liquid and gas phases are essential to accurately and fully describe the system. A crucial aspect is determining the speciation of ions present, as well as their interactions in solution according to the PITZER model. As very low concentrations ($b < 10^{-5}$ mol kgw^{-1}) of CO_3^{2-} and OH^- complexes are expected, specifically tailored analytical methods need to be explored.

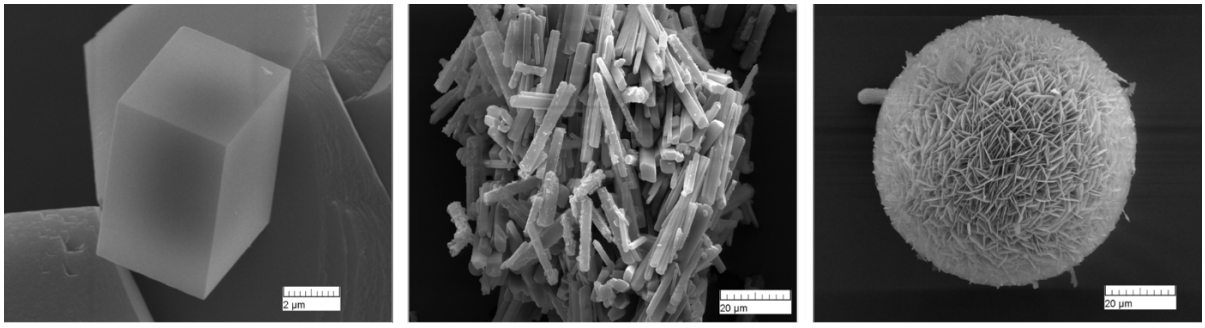

Fig. 1. SEM images of prepared solids; magnesite, nesquehonite, and hydromagnesite.

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EES - D4 - P04

Removal of metallic fragments contained in the waste generated during the manufacturing of photovoltaic cells

Camilia Nafissa Smain[1,2], Sabrina Ridal [2], Nabila Boutouchent-Guerfi [3], Mahdi Derraji [2], Radouan Melouki [2]
[1]Centre de la Recherche et Dévelopement de la Gendarmerie Nationale, Algeria; [2]Unité d'Enseignement et de Recherche en Chimie Appliquée, Ecole Militaire Polytechnique (EMP), Algeria; [3]Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE), Algeria

The photovoltaic panel industry generates a significant amount of slurry during the wafering stage, which involves two main techniques: slurry wire sawing and diamond wire sawing. This process produces effluents rich in pure silicon particles (up to 40%), silicon carbide (SiC), iron (Fe), and polyethylene glycol (PEG). In order to reduce costs and optimize the production of photovoltaic cells, it is crucial to recover and treat this waste.
The effluent was collected and analyzed by FTIR-ATR spectroscopy, highlighting the chemical composition of the PEG lubricant, which was purified for potential reuse. A physicochemical treatment protocol was implemented to separate the liquid and solid phases, with optimization of the washing conditions. The solid phase was characterized by FTIR-ATR and XRD, while the liquid phase underwent thermogravimetric analysis (TGA).
The study of metallic fragments present in the waste was carried out using electron probe microanalysis (EPMA), and dry magnetic separation was explored to remove these fragments. The results allowed for an evaluation of the effectiveness of this separation technique. Finally, the efficiency of this separation technique was assessed by EDX analysis of the magnetic and non-magnetic phases, enabling the identification of the elements present in each phase.

Keywords: Slurry; PEG; Photovoltaic; Metallic fragments; Characterization.

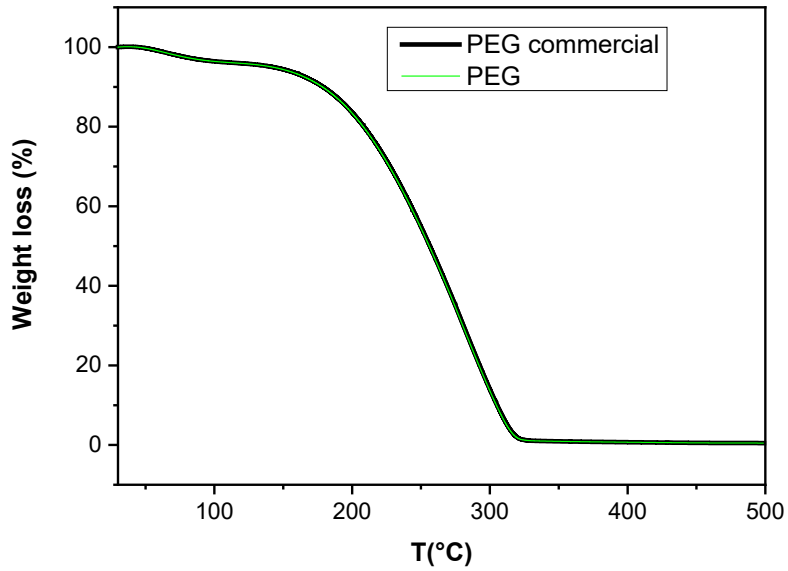

Fig. Thermograms (TGA/DTG) of regenerated PEG and commercial PEG.

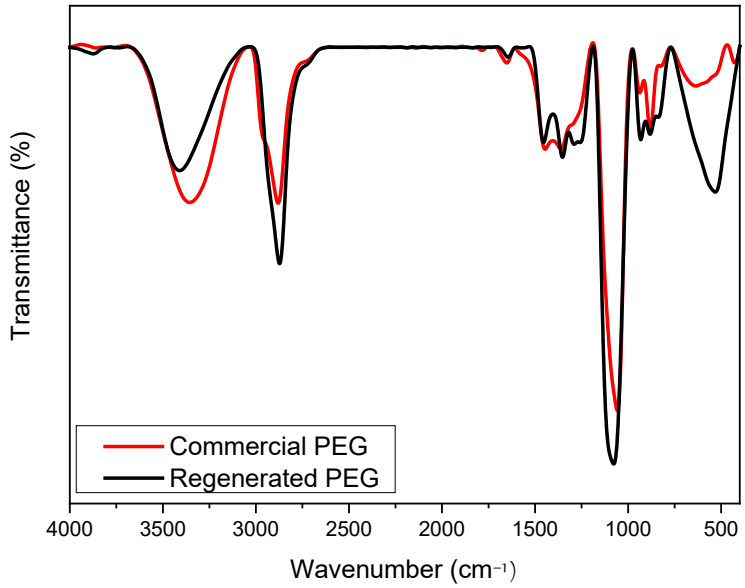

Fig. FTIR-ATR spectra of the liquid phase of regenerated PEG and commercial PEG.

The efficiency of the lubricant was evaluated by characterizing both the regenerated lubricant and the commercial lubricant used as a reference, using FTIR and thermogravimetric analysis (TGA).
The FTIR-ATR spectra of commercial PEG and regenerated PEG were compared. Both spectra exhibit a general similarity, except in the region between 3200 and 3400 cm^{-1}.
In the spectrum of commercial PEG, an intense band is observed in this region, which is likely attributed to the O–H stretching vibration. In contrast, the spectrum of regenerated PEG shows a less intense band, which may correspond to a combination of O–H vibrational modes.

EES - D4 - P05

Identifying complexing agents for the selective binding of Pb^{2+} released during perovskite solar cell degradation

Tia Ansell[1], Rhys G. Charles[1], Rodrigo Garcia-Rodriguez[1], Matthew L. Davies[1,2]
[1]Swansea University, UK; [2]University of KwaZulu-Natal, South Africa

Perovskite solar cells (PSCs) are an exciting, emerging photovoltaic technology showing promise for circular economy applications and contributing to net-zero targets. Currently, PSCs demonstrate power conversion efficiencies up to 27.3 %, aided by a high absorption coefficient and ideal bandgap. However, exposure to moisture, oxygen, heat or light decomposes the Pb-containing perovskite layer into water-soluble lead salts, Pb^{2+}. These species may leach into the environment when modules are damaged during use or end-of-life processing. This leads to harmful accumulation in our biosphere, ultimately impacting human health. To mitigate this, colourimetric methods were explored to assess dyes that selectively bind Pb^{2+}, enabling early detection of PSC degradation and prevention of lead release. Metal–ligand interactions were observed using UV–Vis absorbance alongside visual colour observations to evaluate binding behaviour and complex strength. By binding Pb^{2+} as it forms, these dyes support sequestration while simultaneously offering a visual indication of degradation, creating an approach that reduces environmental emissions and supports real-time monitoring of PSC stability.

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EES - D4 - P06
Comparison of hydrogel coated ion selective solid-state electrodes for nitrate measurements in soil

Thomas Funk[1], Baikun Li[1], Timothy M. Vadas[1]
[1]*University of Connecticut, USA*

Understanding temporal dynamics of nitrate in agricultural soils during different management strategies would help reduce nitrogen leaching to the downstream environment. However, the best methods to examine that are extraction techniques, while *in-situ* measurements are difficult due to variations in moisture content in soils leading to loss of sensor contact with porewater. In order to address this limitation, three hydrogel coatings, acrylamide, lignin and agar, were applied to an established ion selective solid-state electrode for nitrate and compared in terms of linearity of response, range of measurement, and response time for stabilization. All hydrogel options gave reasonable calibrations with Nernst slopes within 20% of ideal in aqueous solution over an extended concentration range of 0-100 mg L NO_3^-N, relevant to agricultural soils. Calibrations in soil mixtures indicated minimal adsorption and loss of nitrate, but the lignin hydrogel resulted in a significant delay in response and reduction in calibration quality, whereas the agar maintained a similar response to aqueous calibration steps (Figure 1). A test was conducted to assess the rate of nitrate diffusion through the hydrogels and time to stabilization and found that the nitrate concentration across the acrylamide did not stabilize within 6 hours, lignin took 4 hours, and agar stabilized within 1 hour. The agar coated ion selective electrode was applied in a moisture controlled soil environment and maintained a valid nitrate reading over the course of a few days in soil at field capacity, but deviated from the measured porewater concentration as soil moisture decreased substantially. Further adjustments to the calibration as a function of soil moisture would help in estimating porewater nitrate concentrations in actual soils.

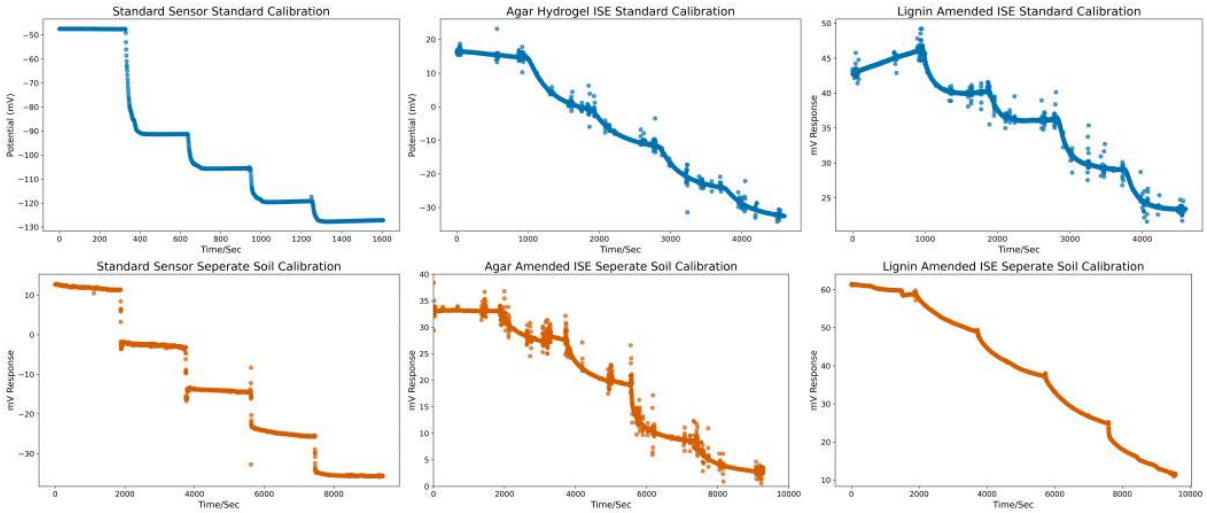


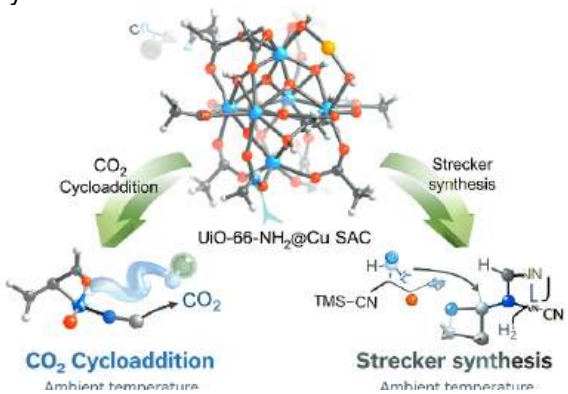
Fig. 1. Calibration comparison of uncoated, agar, and lignin coated ion selective electrodes in solution and soil mixtures.

EES - D4 - P07

Monoatomic copper-anchored UiO-66-NH_2 as a mechanistically defined Lewis acid catalyst for CO_2 cycloaddition and enantioselective Strecker synthesis

Sharad Kumar Sachan[1], Aristides Bakandritsos[1]
[1]Czech Advanced Technology and Research Institute (CATRIN), Regional Centre of Advanced Technologies and Materials (RCPTM), Palacký University Olomouc, Czech Republic

Single-atom catalysts (SACs) have emerged as an advanced class of heterogeneous catalysts due to their maximal atom efficiency and well-defined active sites; however, stabilizing isolated metal atoms while controlling their coordination environment remains a significant challenge [1,2]. In this work, we report a monoatomic copper-anchored metal–organic framework (UiO-66-NH_2@Cu SAC) as a robust Lewis acid catalyst for CO_2 cycloaddition to epoxides and enantioselective Strecker synthesis of α-aminonitriles.
The amine-functionalized UiO-66-NH_2 framework provides strong Cu–N coordination sites that immobilize isolated Cu(II) atoms within the Zr_6-based lattice, generating electronically unsaturated and spatially isolated Lewis acidic centers [3]. In CO_2 cycloaddition, the single Cu site activates epoxides via Lewis acid coordination to the oxygen atom. At the same time, the confined-pore environment facilitates CO_2 insertion and suppresses competing side reactions, thereby achieving high selectivity toward cyclic carbonates [4]. In the Strecker reaction, cooperative activation of imine substrates by isolated Cu Lewis acid sites, combined with steric confinement within the MOF pores, enables efficient stereochemical control, affording α-aminonitriles with high enantiomeric excess. The atomically dispersed Cu sites effectively prevent aggregation and leaching, resulting in excellent catalytic stability and recyclability without loss of activity or enantioselectivity. This study highlights how coordination-defined single Cu sites and confinement effects govern reactivity and selectivity, demonstrating UiO-66-NH_2@Cu SACs as a versatile platform for sustainable CO_2 valorization and asymmetric synthesis.



This work was supported by the **Marie Skłodowska-Curie Actions Postdoctoral Fellowship (MSCA PF)** under the European Union's Horizon Europe programme. The Tech Scale Project provided additional funding.

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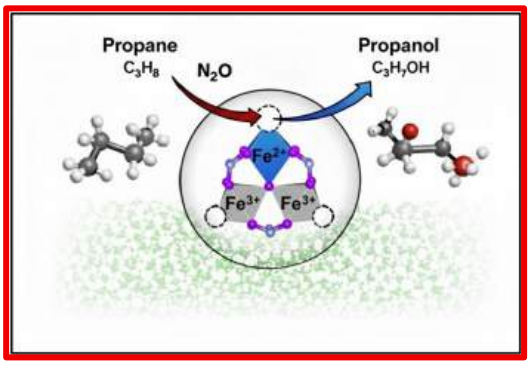
EES - D4- P08

Scale-up, shaping, and catalytic performance of MIL-100(Fe) in propane oxidation

Bezayet Tesfaya[1,2], Barbara Centrella[1], Natale Porcaro[1] Egon Heuson[2] Franck Dumeignil[2] Alessandro Turrina[3], Raquel Garcia[3], Stephen Poulston[3] and Silvia Bordiga[1]

[1]Dept. of Chemistry, NIS and INSTM Reference centre University of Turin, Italy; [2] Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 – UCCS - Unite´ de Catalyse et Chimie du Solide, France; [3]Johnson Matthey Technology Centre, UK

Iron-based metal–organic frameworks (MOFs) are promising catalysts for selective oxidation of light alkanes, but their practical application requires scalable synthesis, suitable shaping, and stable catalytic performance[1,2]. In this study, MIL-100(Fe) synthesis was upscaled (140 g batch) and the product was shaped into pellets and binder-containing granules for operation in a fixed-bed reactor. The synthesized material was shaped into pellets and binder-containing granules to allow operation under industrially relevant conditions[1,3,4]. X-ray diffraction confirmed that the crystalline structure was preserved after shaping. BET surface area measurements showed only a moderate decrease due to mechanical compression and binder addition. SEM–EDX analysis revealed uniform morphology and homogeneous elemental distribution, while thermogravimetric analysis demonstrated unchanged thermal stability. In situ FTIR spectroscopy with CO as a probe molecule confirmed the presence of accessible Fe^{3+} and Fe^{2+} redox sites after activation at 250 °C. Catalytic tests for propane oxidation to propanol were carried out in a fixed-bed reactor. All shaped samples showed stable propanol production with no significant differences in steady-state productivity. These results demonstrate that MIL-100(Fe) maintains its structural integrity and catalytic performance after shaping and is suitable for selective propane oxidation in fixed-bed reactors.



Acknowledgements: This work was carried out within the DEMO project, funded by the European Union's Horizon Europe programme under the Marie Skłodowska-Curie Actions Doctoral Networks (DN) (Grant Agreement No. 101119947).

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EES - D4 - P09

Clay-based platforms for REE recovery: Selective adsorption, regeneration and magnetic separation

Cláudia B. Lopes[1], Giani V. Brião[2], Giovambattista Tomassi[2], Tito Trindade[1], Carlos Manuel Silva[3], Meuris Gurgel Carlos da Silva[2], Melissa Gurgel Adeodato Vieira[2]

[1]Dept. of Chemistry and Aveiro Institute of Materials (CICECO), University of Aveiro, Portugal; [2]University of Campinas – School of Chemical Engineering; [3]CERES- Dept. of Chemical Engineering, University of Coimbra, Faculty of Sciences and Technology, Portugal

Growing technological dependence on rare earth elements (REEs) is driving the search for recovery routes that are both efficient and environmentally responsible. A particularly attractive pathway is adsorption from contaminated waters and leachates produced by industrial operations and mining-related activities, where dilute streams can still represent significant resource value.

This study investigates how naturally abundant clays, notably vermiculite and bentonite, can be progressed from low-cost raw minerals into engineered clay-based nanocomposites for REE capture. We discuss the design logic behind this transition: leveraging clay ion-exchange and surface chemistry, then enhancing performance through functionalisation with spinel ferrite nanoparticles (to enable magnetic separation) and biopolymers (to introduce tailored binding sites), while keeping regeneration and reuse as central requirements. Emphasis is placed on performance in realistic matrices and on practical regeneration strategies.

A central case study focuses on Nd and Dy recovery from end-of-life permanent magnet leachates using expanded vermiculite and vermiculite-derived nanocomposites. Under single-element conditions, raw vermiculite reached sorption capacities of 485 μmol g^{-1} (Nd) and 210 μmol g^{-1} (Dy). In acidic multimetal leachates, uptake followed the sequence Fe > Nd > Zn > Pr > Co > Dy > Ni > Al > Mn, revealing strong competition effects. Although very high total capacities were achieved (up to 12 mmol g^{-1}), selectivity remained limited. For desorption, chelating agents outperformed other eluents, and EDTA showed preferential Nd desorption relative to competing metals, an important result given the difficulty of separating REEs. Post-sorption characterisation indicated that vermiculite largely retained its layered structure, functional groups, chemical composition, and thermal stability.

Overall, clay-based nanocomposites, especially magnetically responsive systems, offer a promising, scalable platform for coupling water remediation with REE recovery, while highlighting that future progress hinges on improving selectivity in complex leachates.

This work was funded by the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) (Grants 2017/18236-1 and 2019/11353-8), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) (Grant 88887.571776 / 2020-00), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) (Grants 406193/2018-5 and 308046/2019-6). This work was also developed within the scope of the project CICECO Aveiro Institute of Materials, UID/50011/2025 (DOI 10.54499/UID/50011/2025) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).Cláudia B. Lopes thanks Fundação para a Ciência e a Tecnologia (FCT) for her researcher contract (CEECIND/03739/2021).

EES - D4 - P10

Activated carbon production from exhaustive olive pomace: Simulation process and autothermal pyrolysis

Jose L. Diaz de Tuesta[1,2*], Cristian Moya[1], Ana Paula Ferreira[3], Helder T. Gomes[3]

[1]Chemical and Environmental Engineering Group, Rey Juan Carlos University, Spain; [2]Instituto de Investigación de Tecnologías para la Sostenibilidad, Rey Juan Carlos University, Spain; [3]CIMO, LA SusTEC, Instituto Politécnico de Bragança, Portugal

The agri-food industry generates large amounts of organic residues whose inadequate management leads to environmental and economic challenges. Exhausted olive pomace (EOP), a by-product obtained after the second extraction of olive oil, is produced in significant quantities in Mediterranean countries and poses particular risks due to its phenolic content, moisture, and high organic load. EOP is an excellent carbon precursor for the production of activated carbon with high uptake capacity [1]. This study investigates the valorization of EOP through its transformation into activated carbon by means of an autothermal pyrolysis process. The objective is to determine whether the system can sustain the thermal energy required for pyrolysis without external heat input under different cases: (1) combusting either a fraction of the raw biomass, (2) part of the resulting biochar, or (3) generated gases. Experimental characterization of real EOP samples was performed using thermogravimetric analysis (TGA) and elemental analysis to determine proximate and ultimate compositions. These results were incorporated into an Aspen Plus V15 simulation framework (Figure 1), where EOP, biochar, and ash were treated as non-conventional components. Results indicate that autothermal operation is feasible in both scenarios; however, combusting biochar is more energy-efficient due to its higher fixed-carbon content and calorific value. Autothermicity is achieved when approximately 43% of the biochar is burned, compared to 14% of the EOP feed. Furthermore, routing the pyrolysis gases to combustion significantly increases net heat production, reaching up to 354 kW versus 36 kW when gases are not recovered. Hydrogen and light hydrocarbons are consistently produced, although their practical valorization would require additional purification steps. Overall, the study demonstrates that EOP can serve as a viable feedstock for activated carbon production via autothermal pyrolysis, offering a sustainable route for waste valorization while ensuring favorable energy balances.

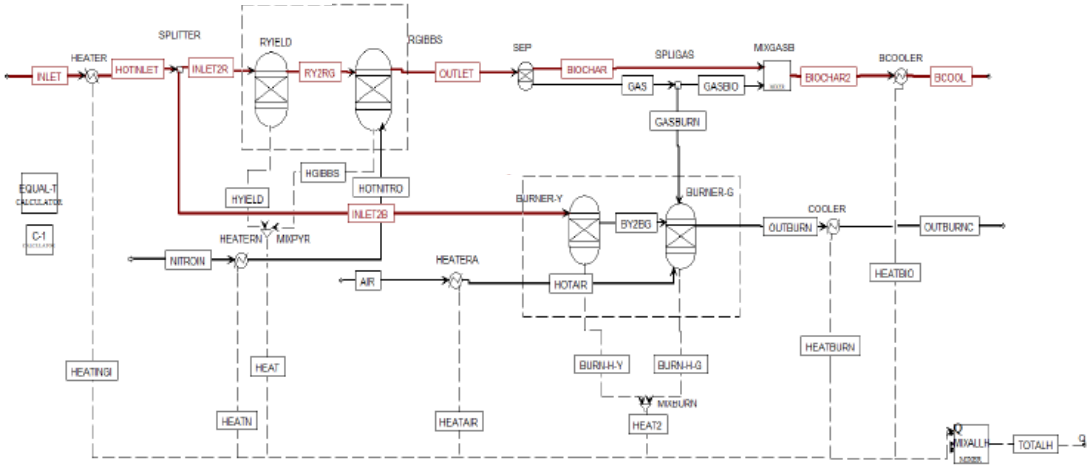

Fig. 1. Main flowsheet diagram of the process (case 1) as viewed from Aspen Plus V15.

Acknowledgements: This work was supported by national funds supported this work through FCT/MCTES (PIDDAC): CIMO, UIDB/00690/2020 (DOI: 10.54499/UIDB/00690/2020) and UIDP/00690/2020 (DOI: 10.54499/UIDP/00690/2020); and SusTEC, LA/P/0007/2020 (DOI: 10.54499/LA/P/0007/2020). Ana Paula Ferreira acknowledges the doctoral Grant PRT/BD/153090/2021 financed by FCT and with funds from NORTE2020, under MIT Portugal Program. Jose L. Diaz De Tuesta acknowledges financial support through the grants 2022-T1/AMB-23946 and CNS2024-154264 funded by *Comunidad de Madrid* and *Agencia Estatal de Investigación*, respectively.

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EES - D4- P11
Synthesis and characterization of lithium metal phosphates in various solvents

Arda Altan[1], Ömer Dağ[2,3]
[1]Bilkent University, Türkiye; [2]Bilkent University, Türkiye; [3]National Nanotechnology Research Center, Türkiye

In this study, lithium metal phosphates (LMPs) are synthesized and characterized using cobalt(II), manganese(II), and nickel(II) nitrate salts. The synthesis is performed using the molten salt-assisted self-assembly (MASA) method. This approach involves forming a lyotropic liquid crystal phase from a clear lithium nitrate ($LiNO_3$), transition metal nitrates ($[M(H_2O)_6](NO3)_2$), phosphoric acid (H_3PO_4), and surfactant (Pluronic P123) alcohol solution. If a resulting solution contains a solid phase, the mixture is subjected to centrifugation to separate into supernatant and solid phases, which are then analyzed using various techniques.

The clear solutions are prepared with molar ratios of 1:30:30:30 (P123:Li(I):M(II):H_3PO_4). Then, they are drop-cast onto glass slides and heated between 300-700°C to form powders. The resulting mesoporous solids formed after calcination are characterized using XRD, SEM, N_2 adsorption-desorption, and ATR-FTIR techniques.

Up to 500°C, the solution, supernatant, and solids remain amorphous but crystallize at higher temperatures. ATR-FTIR analyses reveal that the nitrates in the solution and supernatant decompose by reacting with phosphoric acid. SEM analyses show that the solids became more porous after calcination. N_2 adsorption-desorption analysis indicates that the pore volume and size vary depending on the temperature.

We found that the precipitates form metal pyrophosphates, while the supernatants form LMPs; the supernatants form $LiMnPO_4$, $LiCoPO_4$, and $LiNiPO_4$ in the olivine phase; the precipitates of Mn(II) solution is crystalline $MnPO_4 \cdot H_2O$ that is converted to $Mn_2P_2O_7$ at temperatures above 400°C. The Ni(II) and Co(II) precipitates form $M_2P_2O_7$. Additionally, cyclic voltammetry experiments were conducted at different KOH concentrations. The $LiNiPO_4$ obtained from 1-butanol and coated onto FTO exhibit greater stability and electrochromic properties during water oxidation.

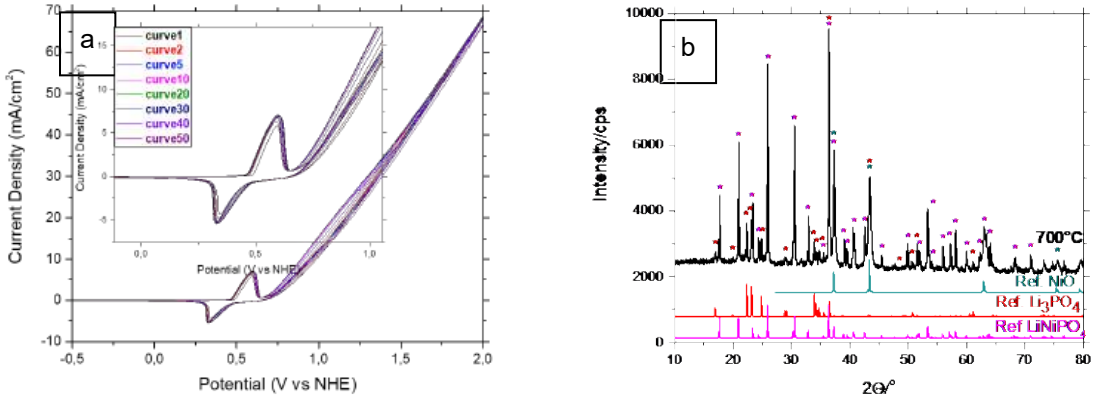

Fig. 1. a) $LiNiPO_4$ electrode (prepared from 1-Buthanol supernatant and calcined at 400 °C), and b) $LiNiPO_4$ supernatant with various crystalls.

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EES - D4- P12

Integrated zeolite membrane and Cu-ZnO-Al_2O_3 catalyst for intensified CO_2-to-methanol conversion

Anamika Maurya, Sweta*, Rajesh Kumar Upadhyay
Indian Institute of Technology (BHU) India
Corresponding Author email: Shweta.che@iitbhu.ac.in

The hydrogenation of CO_2 to methanol is an attractive pathway for carbon utilisation and sustainable fuel production. However, in conventional fixed-bed reactor, Initiate water formation shifts the equilibrium backward, lower methanol yield, and accelerate catalyst deactivation. A membrane reactor integrating a water-selective membrane with methanol synthesis catalyst offers a promising solution for continuously removing water, enhancing conversion via Le Chatelier's principle. This work focuses on development of zeolite membrane and Cu-Zn-Al_2O_3 catalyst and their integration into single membrane reactor system.

The membrane including silicate, zeolite A, zeolite 3A, and ZSM-5 were synthesised on porous alumina support using a secondary growth hydrothermal method. Membrane performance was evaluated through a single and mixed gases permeation experiments, emphasizing H_2O selectivity. It is found that silicate membrane showed lower water transport due to their hydrophobic nature, while ZSm-5 membrane displayed moderate separation behaviours.

Cu-ZnO-Al_2O_3 Catalyst was prepared via co-precipitation with varying total metal loading (10-70 wt.%). Catalytic activity was tested in fixed-bed reactor after calcination and H_2 reduction. Results indicate that metal loading significantly influence methanol productivity: excessive loading led to particle agglomeration and reduced activity whereas intermediate loading improved copper dispersion and enhance CO_2 conversion. Finally, the optimized membrane and catalyst were integrated into a membrane reactor. Reactor performance was evaluated at varying temperature, pressure, and feed flow rate in terms of CO_2 conversion, methanol selectivity and water permeation. Integrated operation showed clear potential for improved methanol yield compared to conventional system.

Acknowledgements: The authors acknowledge the support of the Dept. of Chemical Engineering and Technology, IIT (BHU) Varanasi, for providing research facilities.

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EES - D4 - P13

Kinetic analysis and multiscale hydrolysis of reinforced PET and PBT plastics: Innovative process configurations for enhanced monomer recovery

William de Rezende Locatel[1], Patrick Biller[2]

[1]IFP Energies Nouvelles, France; [2]Dept. of Biological and Chemical Engineering, Aarhus University, Denmark

Plastic use has risen since the mid-20th century due to its durability and versatility. For industrial applications, plastics like Poly(ethylene terephthalate) (PET) and Poly(buthylene terephthalate) (PBT), are often combined with glass fiber to improve mechanical properties. Consequently, recycling these materials is challenging and solvolysis can be considered a viable alternative.[1] The references regarding the chemical recycling of reinforced industrial plastics are scarce, particularly PBT, and effect of glass fiber was not investigated. The novelty of this work lies in a multiscale study of hydrolysis of these materials along with proposing new process configurations to enhance the monomers recovery. First, a kinetic study was performed using data from differential scanning calorimetry (DSC) with high pressure crucibles, a much faster alternative that uses less energy and fewer reagents than batch-scale experiments. We were able to estimate activation energy, identify main trends and eventual side reactions, and the impact of glass fiber on polymeric matrix. Although glass fiber can slightly modify the kinetic parameters, the results from batch experiments showed a small difference in polymer conversion, without impact on the monomer recovery. Furthermore, the batch reactions allowed for the characterization of products obtained and, in the case of PBT, the diol monomer (1,4-butanediol (1,4-BD)) recovery was lower than 10 %, regardless of the presence of glass fiber. To increase the 1,4-BD recovery, we performed hydrolysis in presence of KOH. Under these conditions, the dehydration of 1,4-BD is prevented and its recovery increased from 10% to approximately 80%. For the PET+30%GF it was demonstrated that recycling the process water associated with the washing of solid residues can increase more than 3x the initial concentration of EG without an impact on polymer conversion, as represented on Figure 1.

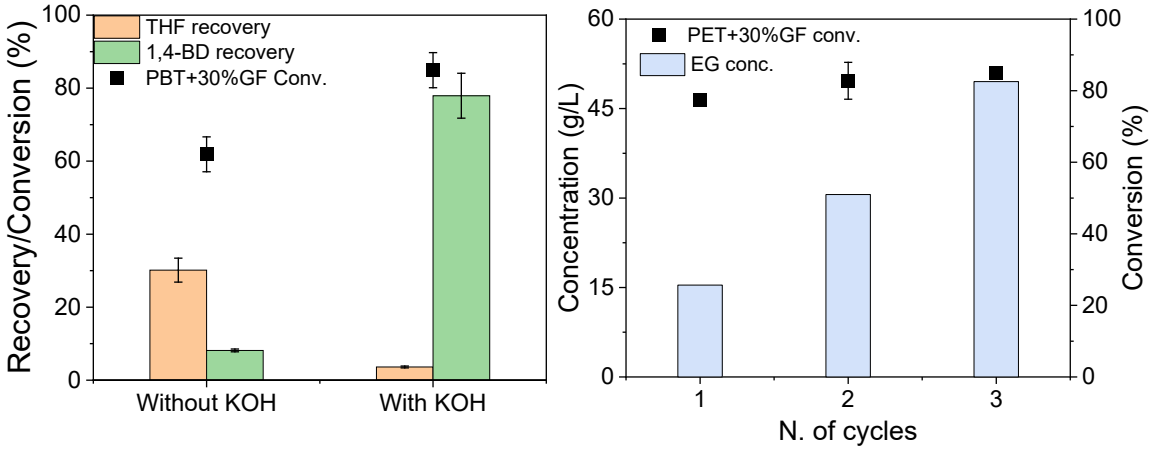

Fig. 2. Conversion and monomer recovery for various strategies to enhance monomer recovery in PBT (left) and PET (right) reinforced with 30% glass fiber.

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EES - D4 - P14
Electroreduction of CO_2 to C1 and C2 products on dual active sites

Naimat Ullah, Munzir H. Suliman, Muhammad Usman
Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia;

Electrochemical CO_2 reduction (eCO_2RR) is a promising method for transforming CO_2 emissions into useful multicarbon products. This study involved the synthesis and evaluation of CuS/ZnS nanocomposites with varying compositions (CuS: ZnS = 1:1, 2:1, and 1:2) in both H-type and flow-cell electrolyzers. The catalyst with a 2:1 CuS/ZnS ratio (S2) exhibited excellent performance, with a Faradaic efficiency (FE) of 60% for C_1 products and approximately 20% for C2 products (C_2H_4) at a current density of −280 $mA \cdot cm^{-2}$ in the flow-cell configuration. The flow-cell arrangement significantly enhanced catalytic activity, suppressed hydrogen evolution, and increased selectivity for CH_4 and C_2H_4 at greater negative potentials. Augmented ethylene production was ascribed to Cu-rich active sites promoting efficient C–C coupling and increased CO_2 accessibility at gas diffusion electrodes (GDEs), corroborated by low charge-transfer resistance (~1 $\Omega \cdot cm^2$). This work emphasizes the pivotal importance of catalyst composition and reactor design, showcasing the 2:1 CuS/ZnS catalyst in a flow-cell format as a scalable and effective method for sustainable CO_2 conversion to multicarbon fuels. Density functional theory (DFT) calculations further validated the experimental results by revealing favorable adsorption energies and interactions between the CuS/ZnS catalyst and key intermediates in the CO_2 conversion process.

EES - D4- P15

Efficient dissolution and selective recovery of gold from electronic waste using a recyclable ionic medium

Abhijit Nag[1]*, Abinash Swain[2], Mudila Dhanunjaya Rao[3], Jacob Lynge Elholm[1], Vitor A. S. Almodovar[1], Rohit B Meshram[3], Pankaj Bharmoria[1], Helen Hölzel[1,4], Kamalesh K Singh[5], Guillem Aromí[2], Kasper Moth-Poulsen[1]*

[1]Universitat Politècnica de Catalunya, Spain; [2]Universitat de Barcelona, Spain; [3]CSIR- National Metallurgical Laboratory, India; [4]Justus-Liebig-Universität Giessen, Germany; [5]Indian Institute of Technology (Banaras Hindu University), India

**Corresponding author*

The significant socio-economic and technological importance of gold necessitates sustainable supply to meet the continuously rising demand. As the demand rises, recovering gold from secondary sources has become increasingly important, highlighting the need for environmentally and economically sustainable extraction processes.[1-5] In this study, gold was efficiently and rapidly leached quantitatively as Au(III) halometalate (Cl/Br) complexes and selectively recovered (~100%) in eight different hydrophobic ionic liquids (ILs) based on pyridinium, pyrrolidinium, and imidazolium at room temperature from both mixed metals solution and electronic waste (e-waste). ILs were recovered after extraction, and used for another two cycles for dissolution and recovery of gold thus demonstrating the economic sustainability of the developed process. Moreover, a techno-economic analysis of the method reveals attractive numbers for gold recovery, even without recycling of ILs. The background for the selective chemistry was studied comprehensively using diverse analytical techniques, complemented by density functional theory (DFT) calculations, and life cycle analysis (LCA). Furthermore, single crystal X-ray diffraction and DFT calculations revealed that non-covalent interactions between the cationic part of the IL and Au(III) halide are key for selective gold separation. The LCA study demonstrates that the process can lower CO_2 emissions by ~84.4% compared to conventional gold mining under the current Indian energy mix, with the potential for an almost complete emissions reduction (~99.9%) if powered by solar energy. The developed process is expected to pave the way for economic and environmentally sustainable recycling of multi-metals from e-waste.

Acknowledgements: A.N. and K.M.P. acknowledges the Marie Skłodowska-Curie Actions–European Commission post-doctoral grant (REWCHEM, Grant agreement ID: 101152892) and Sustain-a-Print project (Grant agreement ID: 101070556) from European Commission for research funding. P. B. acknowledges, Ramón y Cajal grant from Spanish State Investigation Agency (Grant no. J03416).

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EES - D4 - P16

Comparative assessment of microplastic accumulation in upper catena fisheries of the Kothmale reservoir, Sri Lanka

H.N.L. Jayasekara[1], D.S.M. De Silva[1], A.A.D. Amarathunga[2], C.N. Walpita[3], S.R.C.N.K. Narangoda[2]
[1]Dept. of Chemistry, University of Kelaniya, Kelaniya, Sri Lanka; [2]Environmental Studies Division, National Aquatic Resource Research and Development Agency (NARA), Crow Island, Sri Lanka;
[3]Dept. of Livestock Production, Faculty of Agricultural Sciences, Sabaragamuwa University of Sri Lanka, Sri Lanka

Microplastic (MP) pollution has rising threats in environmental safety. This study aims to address the gap in MP contamination of upper catena freshwater fish in Sri Lanka by examining MP accumulation in three fish species, *Rasbora microcephalusv, Glossogobius giuris and Puntius dorsalis* inhabiting in the Kothmale reservoir, Sri Lanka. Samples (n = 75) were collected from the local fishermen in July and October 2024. Samples were digested in 10% KOH, stained with Nile red, identified under a stereomicroscope, and further by the μ-FTIR spectroscopy. Overall, MPs were detected in 52% tracts (n =39) and 37.3% gills (n=28). In *R. microcephalusv,* the mean MP abundance was 0.039 ± 0.042 items/gram. Fibers are dominated (64%), while most frequent MP size range (0.1 - 1 mm) accounted for 77.27%. Predominant colors of MPs were blue, black, and red, with blue at 56%. In *G. giuris,* mean MP abundance was 0.012 ± 0.010 items/gram. Fibers have dominated (88%) with the most MPs sized 0.1 - 1 mm (52.38%) in range. Blue, black and red colours MPs were prevailed, with blue colour comprising in 46%. In *P. dorsalis,* the mean MP abundance was 0.062 ± 0.071 items/gram with fibers constituting 63%. Most MPs were sized 0.1 - 1 mm (90.70 %), with blue making up 74%. The chemical composition of extracted MPs from fish samples revealed Polyolefin fibers, HDPE, Polypropylene (PP). There was a significant difference between three species ($p < 0.05$). Findings indicate broad MP pollution, needing better monitoring to prevent harm.
Keywords – Microplastic, Rasbora microcephalus, Glossogobius giuris, Puntius dorsalis, μ-FTIR

Acknowledgement: Financial assistance received from the Association of Commonwealth Universities (ACU) under the Ocean Country Partnership Programme (OCPP) of the Blue Planet Fund and University of Kelaniya and Laboratory facilities from the National Aquatic Resources Research and Development Agency (NARA) are acknowledged is acknowledged.

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EES - D4 - P17

Tailored-shell hollow TiO_2 spheres with reduced tortuosity for fast-charging anode

Sangeun Chun[1,2,3,*], Chang-Wan Hyeon[1,2,3], Chan Woo Kim[1,2,3]

[1]School of Materials Science and Engineering, Kyungpook National University, Republic of Korea; [2]Innovative Semiconductor Education and Research Center for Future Mobility, Kyungpook National University, Republic of Korea; [3]Research Institute of Automotive Parts and Materials, Kyungpook National University, Republic of Korea

Growing attention has been paid to next-generation anode materials beyond graphite. Titanium dioxide (TiO2) has attracted considerable interest due to its structural stability and natural abundance; however, its practical application is limited by sluggish Li^+ transport arising from the dense arrangement of TiO_6 octahedra.

In this study, we present a structurally engineered TiO2 anode featuring a hollow mesoporous architecture composed of nanoscale anatase particles. The design integrates two key advantages: (i) a shortened Li+ diffusion pathway enabled by thin shells and (ii) enhanced electrolyte accessibility through interconnected mesopores. The hollow interior further provides additional active interfaces, allowing bidirectional ion transport across the shell.

The hollow TiO2 spheres were synthesized via a template-assisted route, where sub-20 nm TiO2 nanoparticles prepared by a sol-gel process were assembled onto carbon nanospheres, followed by removal of the sacrificial carbon core. By precisely controlling shell thickness, the ion transport resistance within the electrode was significantly reduced while suppressing isolated pore formation. As a result, a Li+ diffusion coefficient of 3.22x10-11 cm2 s-1 was achieved, representing a ~40-fold enhancement compared to bulk TiO2.

Electrochemically, the optimized TiO2 anode delivered 0.66 mol Li per mol TiO2 at 0.5C and retained 67% of its capacity even at 10C, demonstrating excellent rate capability. In addition, long-term cycling at 20C exhibited a capacity retention of 85.9% over 1000 cycles, indicating outstanding structural robustness under high-rate conditions. When paired with a LiFePO4 cathode, the full cell showed a rate performance of 60% (2000 vs. 50 mA g-1, surpassing that of conventional bulk TiO2 systems.

These results highlight that rational control of mesostructure and shell thickness is an effective strategy to overcome intrinsic kinetic limitations of TiO2, providing a viable pathway toward high-power lithium-ion batteries.

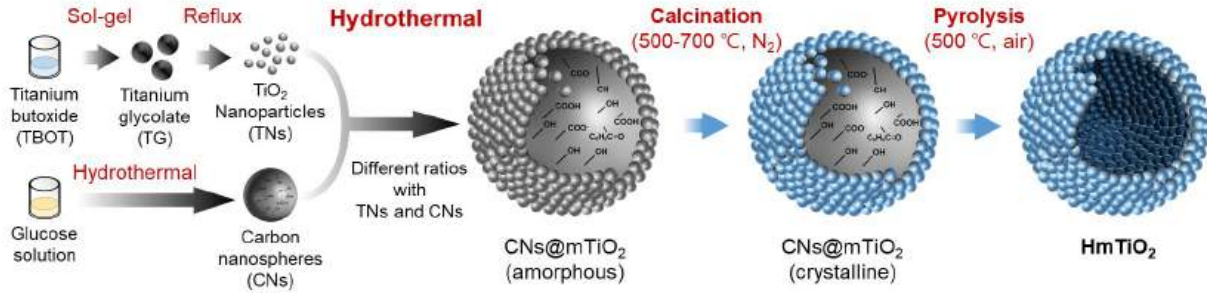


Fig. 1. Schematic of the synthesis of hollow mesoporous TiO_2 spheres ($HmTiO_2$) using carbon nanosphere as a sacrificial scaffold, onto which TiO_2 nanoparticles were assembled, followed by calcination and pyrolysis.

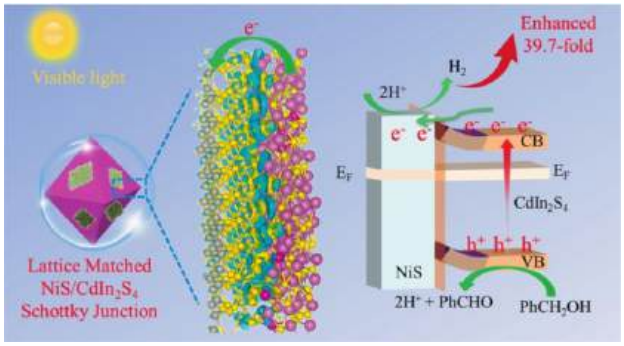
This work was supported by the National Research Foundation of Korea (NRF) funded by the Korean government (Ministry of Science, ICT & Future Planning) (NRF-2021R1A4A2001658; NRF-2022R1A2C1009922).

EES - D4 - P18

Regulating redox sites for photocatalytic phenylcarbinol conversion and H_2 production on lattice-matched Schottky junction

Fengqin Wang[1], Xinyue Ren[2], Yang Wang[1,*], Muhammad Tayyab[3,*], Zhongliao Wang[2], Sugang Meng[2,*]
[1]*School of Mechanical Engineering, Nantong Institute of Technology, Nantong, Jiangsu 226006, P. R. China;* [2]*Key Laboratory of Green and Precise Synthetic Chemistry and Applications, Ministry of Education, School of Chemistry and Chemical Engineering, Huaibei Normal University, China;* [3]*Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals, Saudi Arabia*

The photocatalytic coupling of selective phenylcarbinol oxidation with hydrogen evolution has attracted considerable attention as a promising dual-functional reaction system. Herein, a lattice-matched 2D/3D NiS/$CdIn_2S_4$ (NiS/CIS) Schottky heterojunction is rationally designed for efficient dual-functional photocatalysis under visible light. Structural analyses confirm the uniform deposition of NiS nanosheets on octahedral CIS with a lattice mismatch below 5%, ensuring coherent interfacial contact. The optimal 3% NiS/CIS composite exhibits exceptional hydrogen and benzaldehyde production rates of 2636.4 and 2717.6 μmol g^{-1} h^{-1}, respectively—representing enhancements of 39.7 and 38.0 times over pristine CIS. The catalyst also demonstrates remarkable stability, retaining over >99.0% activity after six cycles. Mechanistic studies reveal that the Schottky junction facilitates spatial separation of photogenerated carriers: electrons migrate to NiS, prolonging charge carrier lifetimes and lowering the hydrogen evolution overpotential, while holes accumulate on CIS that facilitated phenylcarbinol adsorption to drive selective phenylcarbinol oxidation via a carbon-radical pathway. This work provides a viable approach for designing efficient bifunctional photocatalysts through lattice-matched interface engineering.



Graphic abstract: Lattice-matched 2D/3D NiS/$CdIn_2S_4$ Schottky junction was designed and prepared for efficiently separation and guided transfer of photogenerated electrons and holes into targeted redox sites, leading to efficiently and sustainably dual-functional photocatalysis.

EES - D4 - P19
Revealing battery interface chemistry with spectroscopy

Matthijs Holthuijsen[1,2], Frederik Huld[2], HanHo Lee[2], David S. Hall[1]
[1]Dept. of Energy and Petroleum Engineering, University of Stavanger, Norway; [2]Beyonder AS, Norway

Interfaces and interphases largely determine the lifetime, performance, and safety of modern commercial lithium-ion batteries. Yet, probing the formation and chemical composition of these thin and unstable "solid-electrolyte interphases" (SEIs) remains very difficult. As a result, the battery cell conditioning protocols used in industry to establish a "good SEI" are often lengthy and expensive, guided by institutional knowledge and historical practice, rather than chemical considerations. In this work, we present an analytical toolkit that can be used to track the generation and evolution of these interphases: Operando shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS), and post-mortem Nuclear Magnetic Resonance (NMR) spectroscopy. The methods are demonstrated with standard 2032-format coin cell batteries constructed with commercial lithium-ion battery electrodes and a model electrolyte. Data will be presented addressing a longstanding dispute[1-4] regarding the chemical composition of an SEI layer forming on a graphite anode with an electrolyte containing ethylene carbonate. The origin of this dispute is traced to moisture contamination and the formation of metallic lithium depositions, both of which were found to alter the chemical structure of the carbonate-based decomposition products that dominate the SEI. It is hoped that these insights will aid in the development of better batteries and cell conditioning protocols in the future.

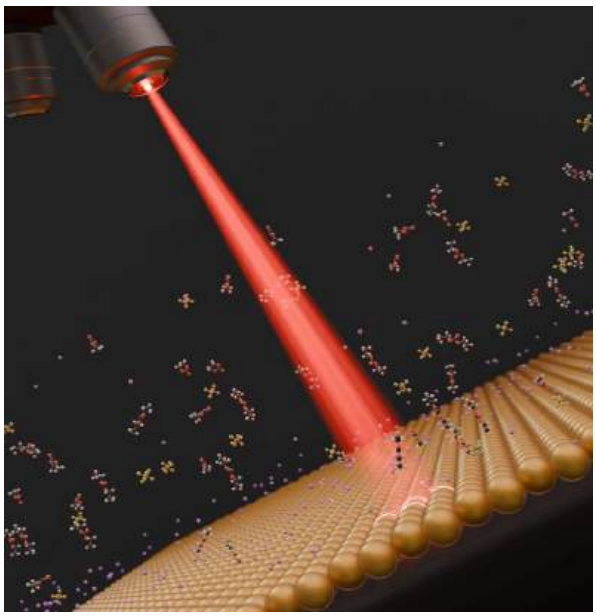


Fig 1. Illustration of the SHINERS method on a graphite anode.

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EES - D4 - P20
Investigation of MOF Derived NASICONs for capacitive deionization application

Ali Furkan Albora[1], Aslı Sare Gürsu[1], Şahika Sena Bayazit[1]
[1]*Institute of Nanotechnology and Biotechnology, İstanbul University-Cerrahpaşa, İstanbul, Türkiye*

Global water scarcity necessitates the development of highly energy-efficient desalination technologies. While Capacitive Deionization (CDI) stands out as a sustainable alternative, the system's efficiency is directly dependent on the electrochemical properties of the electrode materials[1]. This study investigates the synthesis and performance of NASICON-type structured materials derived from Metal-Organic Frameworks (MOFs) for the selective removal of Na ions from brackish water. By using MOFs as sacrificial templates, a hierarchical porous architecture that facilitates rapid ion diffusion and offers a high surface area has been successfully designed. Through the carbonization of MOF precursors followed by thermal treatments, a stable NASICON framework (e.g., $Na_3Zr_2Si_2PO_{12}$ or similar analogs) integrated into a conductive carbon matrix has been obtained. This unique structure preserves structural integrity while simultaneously leveraging the high theoretical capacity of faradaic materials. Electrochemical evaluations, including cyclic voltammetry and galvanostatic charge-discharge tests, demonstrate that MOF-derived NASICON electrodes exhibit higher salt adsorption capacity (SAC) and faster desalination kinetics compared to conventional activated carbon electrodes. This performance improvement is based on the synergistic effect between the intercalation pseudocapacitance of the NASICON phase and the high conductivity of the MOF-derived carbon. In this study, MOF crystals obtained from titanium salt and dihydroxyterephthalic acid will be converted into NASICON. And the prepared electrodes using for desalination of seawater. This research presents a promising strategy for the design of next-generation, high-performance electrodes for efficient water treatment.

Acknowledgement: This work was supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) under grant number 223M289.

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EES - D4 - P21

Proposal for restriction on difluoromethylene substances aka “universal PFAS restriction”: Chemical analysis

Vladimir Nikiforov
NILU, Norway

Currently considered proposal for restriction of “Per- and polyfluoroalkyl substances (PFAS)”[1], does not define the restricted compounds correctly. A reasonably correct chemical name could be, for example, “substances with at least one difluoromethylene group, not connected to H, Cl, Br of I”.
The name “PFAS” is confusing: a substance with a -CF_2- may be not an “alkyl” substance (Fig. 1).
The formula for exclusion of certain “PFAS” from the restriction – “A substance that only contains the following structural elements is excluded from the scope of the proposed restriction: CF3-X or X-CF2-X’, where X = -OR or -NRR’ and X’ = methyl (-CH3), methylene (-CH2-), an aromatic group, a carbonyl group (-C(O)-), -OR’’, -SR’’ or –NR’’R’’’, and where R/R’/R’’/R’’’ is a hydrogen (-H), methyl (-CH3), methylene (-CH2-), an aromatic group or a carbonyl group (-C(O)-).” - is as complex as controversial and, therefore, hardly of any use: each mentioned substance of formula X-CF_2-F can be considered as X-CF_3 or as X-CF_2-F’, with the opposite outcomes (Fig. 1).
For an organic chemist, it is hard to understand why only ethers of primary alcohols are suggested for exclusion, while equally degradable ethers of secondary and tertiary alcohols – not (Fig. 1).
For an environmental chemist, it is hard to accept more severe restrictions on substances with difluoromethylene group, and milder restrictions on substances with “more perfluorinated” trifluoromethyl group (Fig. 1).
These inconsistencies originate from the report[2] with explanation of “PFAS” for non-experts, which was later presented as “A New OECD Definition for Per- and Polyfluoroalkyl Substances” in a non-peer reviewed paper[3] and laid foundation for the restriction proposal.
Use of scientifically correct description of substances proposed for restriction, instead of excerpts from non-peer reviewed papers should be recommended in the future, to avoid science-based criticism and enhance credibility of environmental protection initiatives.

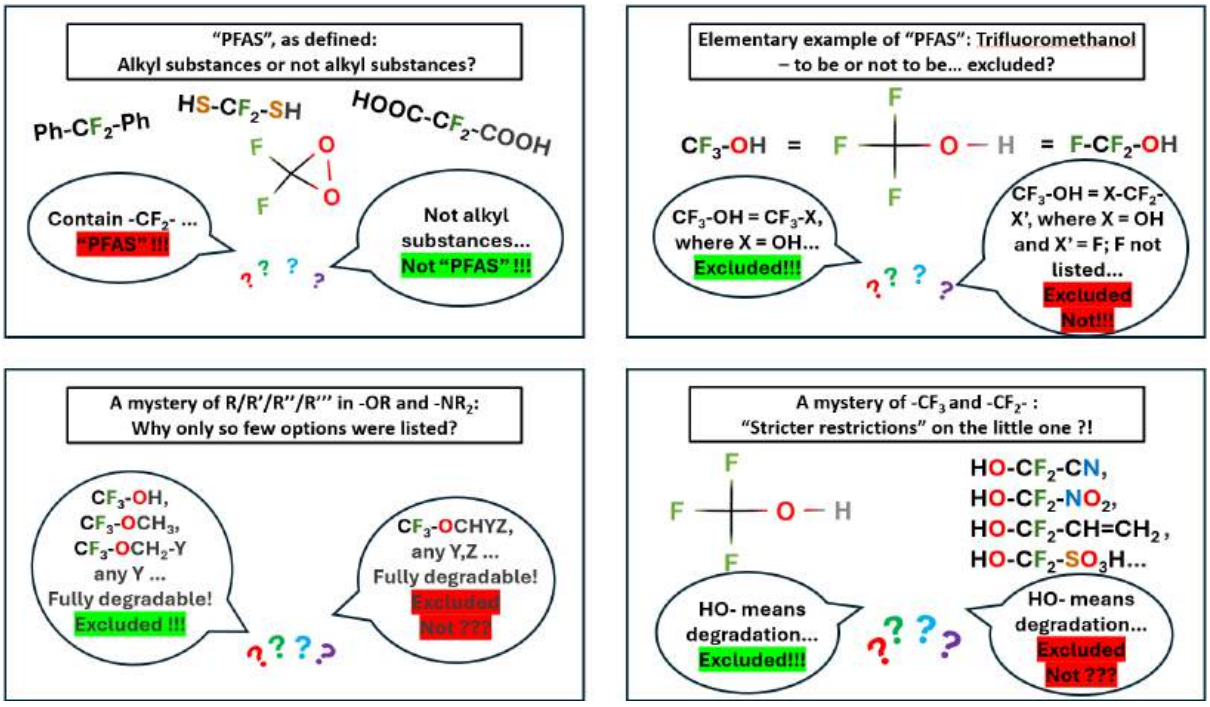

Fig. 1. Graphical representation of major inconsistencies of the restriction proposal.

[1]Registry of restriction intentions until outcome - ECHA
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EES - D4 - P22

Electronic structure engineering via atomic W doping in NiO/Cr_2S_3 nanotube heterostructures for enhanced overall water splitting

Mai Mai[1], Van Hien Hoa[2], Do Hwan Kim[1,3]

[1]Dept. of Energy Storage/Conversion Engineering, Jeonbuk National University, Republic of Korea; [2]Dept. of Nano Convergence Engineering, Jeonbuk National University, Republic of Korea; [3]Dept. of Chemistry Education, Jeonbuk National University, Republic of Korea

The development of durable and highly active non-precious electrocatalysts for hydrogen and oxygen evolution reactions (HER/OER) is essential for advancing hydrogen energy technologies. Herein, we report a vertically aligned W-doped NiO/Cr_2S_3 nanotube heterostructure grown on nickel foam (denoted as $W–NiO/Cr_2S_3/NF$) via a combined electrodeposition and etching strategy. The incorporation of W atoms effectively modulates the electronic structure of the NiO/Cr_2S_3 interface, leading to enhanced intrinsic catalytic activity. Density functional theory (DFT) calculations reveal that the HER activity is governed by the electronic states of the active valence dz^2 orbitals. W doping introduces antibonding states with an optimized occupancy, resulting in near-ideal hydrogen adsorption energetics. As a result, the $W–NiO/Cr_2S_3/NF$ electrode exhibits outstanding bifunctional catalytic performance for overall water splitting, requiring a low cell voltage of 1.58 V at 10 mA cm^{-2}. Moreover, it demonstrates excellent durability over 50 h in 1.0 M KOH, surpassing the performance of commercial Pt/C and IrO_2 catalysts. These findings highlight the effectiveness of atomic-level doping in tuning electronic structures and provide a promising strategy for designing high-performance electrocatalysts for sustainable hydrogen production.

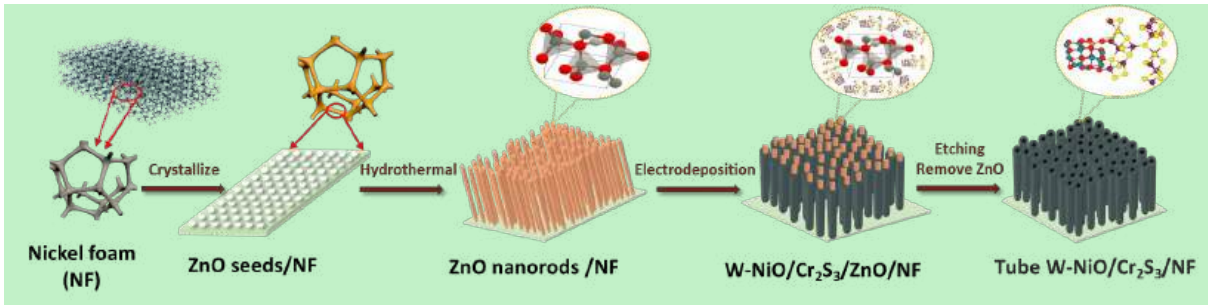

Fig 1. Material Fabrication: W-doped NiO/Cr2S3 hollow heterostructure on nickel foam

Acknowledgement: This work was supported by the Korea-Vietnam Joint Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2026-16063221). This research was also supported by the Regional Innovation System & Education (RISE) program, funded by the Ministry of Education (MOE) and the Jeonbuk State, Republic of Korea (2025-RISE-13-JBU).

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EES - D4 - P23
Ti/Fe-based MOF photocatalysts for efficient solar-driven dye removal

İrem Doğruyol, Beste Erüstün, Çisem Devrim Değirmenci, Utku Öztürk, Özge Kerkez Kuyumcu*
Marmara University, Faculty of Engineering, Chemical Engineering Dept., Türkiye

The discharge of dye-containing wastewater poses a significant environmental challenge due to its toxicity, persistence, and resistance to conventional treatment methods. In this context, solar-driven photocatalysis has emerged as a sustainable and energy-efficient alternative for the degradation of organic pollutants [1, 2]. This study focuses on the synthesis and evaluation of Ti/Fe-based metal–organic framework (MOF) photocatalysts for the efficient removal of dye contaminants under solar irradiation.
Ti-MOF, Fe-MOF, and bimetallic Ti/Fe-MOF structures with different metal ratios were synthesized and systematically characterized in terms of their structural, morphological, and optical properties. The photocatalytic performance of the prepared materials was investigated using methylene blue as a model dye pollutant under simulated solar light.
To optimize the degradation process, a Taguchi L16 experimental design was employed. Four key factors—catalyst type, catalyst loading, initial dye concentration, and reaction time—were examined at four levels each. This approach enabled the identification of the most influential parameters affecting photocatalytic efficiency with a reduced number of experiments. The experimental results were statistically analyzed using analysis of variance (ANOVA) to determine the significance and contribution of each factor. The findings highlight the potential of Ti/Fe-based MOF photocatalysts as promising candidates for sustainable wastewater treatment applications.

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EES - D4 - P24
Fine-tuning the supercapacitor's performance with EPR spectroscopy

Ameen Uddin Ammar[1], Angela M. Kasza[1,2], Maria Mihet[1], Arpad M. Rostas[1]
[1]National Institute for Research & Development of Isotopic and Molecular Technologies, Romania;
[2]Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania

Supercapacitors (SCs) are promising energy storage devices, where the electrode materials are key components; selecting the right electrodes is crucial to their specific power and energy storage performance. 3D carbon materials derived from MOFs and impregnated with ZnO are used as electrode materials in hybrid SC devices. Here, their electrical properties are enhanced by controlling and tailoring the size, shape, defects, interfacial phenomena, and porosity of the materials' nanostructures. The high-sensitivity EPR spectroscopy method is used to characterize defect structures, including carbon-related defects and oxygen-vacancy-related defects, in ZnO. The characterization by spectroscopic techniques on the surface and interface of the electrodes and their influence on the electronic, optical, and electrical properties of the nanocomposites is carried out to improve the properties of the material, so that new SC electrodes in a solid-state configuration using a 3D-carbon structure/ZnO are obtained to improve the energy storage capacity.

Acknowledgement: The authors acknowledge the support of a grant from the Ministry of Research, Innovation and Digitization, CNCS—UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0048, within PNCDI IV.

EES – D4 - P25
Valorisation of waste tea leaves and egg shells in carbon nanodot synthesis

Ecem Bayram[1], Ummuhan Arabaci[1], Asude Sena Demirci Ulke[1], Yasar Andelib Aydin[1]
[1]Marmara University, Chemical Engineering Dept., Turkiye

Utilization of food waste as renewable raw materials offers vast opportunities in terms of tbioeconomy and the reduction of associated environmental concerns1. Concordantly, significant research effort has been put into the valorisation of food waste to create 'added value products' such as carbohydrates, essential oils, enzymes[2], and even nanomaterials, particularly carbon nanoparticles and carbon quantum dots (CNP, CQD)[3]. The exquisite optical, electrical and chemical properties of CQDs facilitate their utilization in a variety of applications ranging from sensors, and bio-imaging to food packaging and water treatment[3].
In this study, waste tea leaves and eggshells were utilized as low-cost raw materials for the synthesis of carbon nanodots (CNDs). While tea wastes served as the primary carbon source due to the inclusion of carbonaceous organic compounds, eggshells acted as a dopant and modifier due to the abundancy of calcium carbonate in its structure.The synthesis was conducted solvothermally in a deep eutectic solvent composed of urea and glycerol. The effects of solvent composition, reaction temperature and precursor ratio on CND properties and yield were evalutaed. The chemical, optical and moprhological characteristics of CNDs were determined using UV–Vis absorption spectroscopy, fluorescence spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and transmission electron microscopy (TEM).
The results verified nanoparticle formation with photoluminescent character. Reaction temperature was identified as the most effective parameter. The presence and density of hydroxyl and carboxyl surface functional groups were also affected, which determined water solubility. Moreover, increased ratio of eggshells led to enhanced optical properties.

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EES - D4 - P26
Bioinspired catalysts for photoelectrochemical solar energy conversion

Corentin Pigot [1], Simona Porzio[2], Sergii Shyliin[3]

Employing renewable energy for the production of green fuels, using atmospheric CO_2 as building block, is one of today's greatest technological challenges. Fossil resources have had a monumental impact on the quality of life during the past century, with an abundance of commodities such as fuels and chemicals being produced for the enrichment of everyday life. High shares of fuels from non-fossil origin are needed by 2050, if the target for net-zero emissions should be reached [1]. Nowadays, eFuels can be produced by electrocatalytic water oxidation and CO_2 reduction. However, rare and expensive metals are required, and catalysts have low stability and are sensitive to poisoning. In addition, production of eFuels relies on the external electricity input from intermittent sources [2].

In this project, **we are working on a technology inspired by photosynthesis, where solar energy is converted directly to fuels without secondary energy carriers**, such as external renewable electricity generated *e.g.* with separate photovoltaics (PV). In the process of direct solar-to-fuel (STF) production proposed here, the energy from sunlight is used to oxidize water into oxygen (O_2), and released electrons are used to reduce CO_2 to various fuel targets. **Our vision** is to develop a photoelectrochemical (PEC) cell technology for direct STF conversion. **The unique feature of this project is the combination of molecular catalysts for water oxidation and CO_2 reduction with light absorbing semiconductors.**

In this system the catalysts are made out of Cu, Fe or Ni which are extremely robust in water in both low and high oxidation states [3,4]. In combination with a relatively low water oxidation overpotential [4], this makes this family of materials excellent WOCs, which hold the promise to compete with the well-known Ru- and Ir-based catalysts [4].

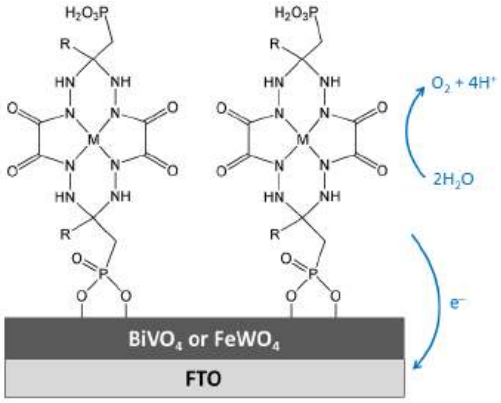

Figure 1. *Photoanode containing new tetrahydrazido complexes as WOCs (M = Mn, Fe, Cu, Fe).*

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EES - D4 - P27

Atmospheric microplastics in a Brazilian elementary school and true-to-life PET-associated internalization and mitochondrial dysfunction in lung-relevant models

Gabriel Ferraz,[1,2] Gustavo Bitencort,[1] Laia Pareras,[2] Santi Trischitta,[2,3] Javier Gutiérrez,[2] Alba Hernández,[2] Laura Rubio,[2] Roberta Urban[1*]

[1]Federal University of São Carlos, São Carlos, Brazil; [2]Autonomous University of Barcelona, Barcelona, Spain; [3]University of Messina, Messina, Italy

Airborne micro and nanoplastics (MNPs) are emerging inhalation hazards, yet their occurrence in school environments and associated biological effects remain poorly understood.[1] This study combined the environmental characterization of atmospheric MNPs in a Brazilian elementary school[2] with a preliminary toxicological evaluation of a representative true-to-life polyethylene terephthalate (PET)[3] material in lung-relevant in vitro models. Atmospheric MNPs were detected indoors and outdoors, ranging from LOD to 60.16 items m^{-2} day^{-1} indoors and from LOD to 168.03 items m^{-2} day^{-1} outdoors. Particles were predominantly fragments, and μ-Raman analysis identified polyester as the major component, with ethylene vinyl acetate (EVA), polyethylene (PE), and PET also detected (**Figure 1**).

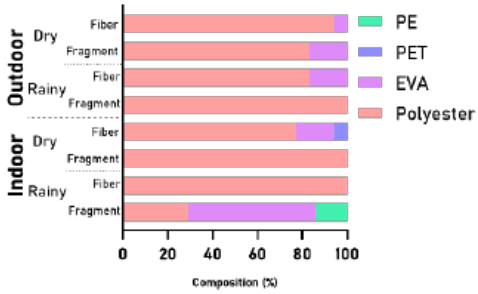

Fig. 1. Polymer composition of atmospheric microplastics and nanoplastics collected in indoor and outdoor environments of a Brazilian elementary school.

To investigate PET-associated cellular responses in lung-relevant systems, differentiated THP-1 (dTHP-1) cells and a Calu-3/dTHP-1 co-culture barrier model were exposed to a representative true-to-life PET material for 24 h. Qualitative confocal microscopy showed PET-associated signal in dTHP-1 cells and in the co-culture, while orthogonal views supported particle-associated localization in both macrophage-like and epithelial compartments (**Figure 2**).

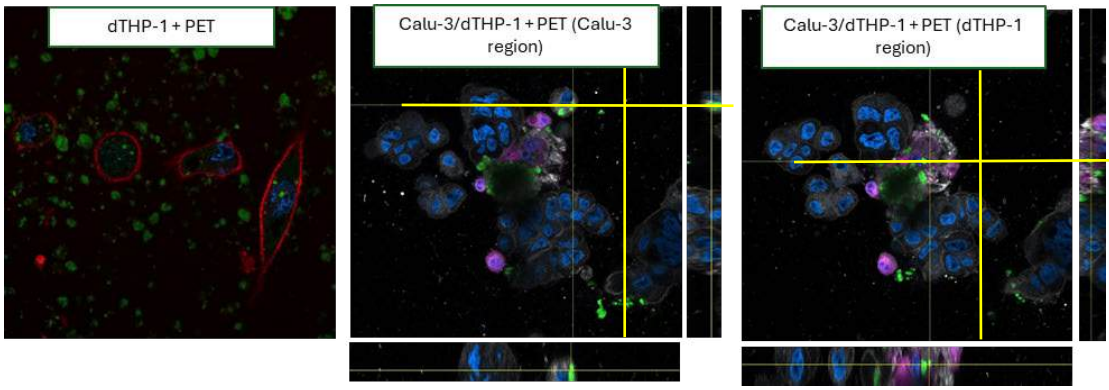

Fig. 2. Confocal images of dTHP-1 and Calu-3/dTHP-1 co-culture after 24 h exposure to PET. Cell membrane, white; nuclei, blue; dTHP-1 cytoplasm, magenta; PET-associated iDye signal, green

Mitochondrial effects were then assessed in the Calu-3/dTHP-1 co-culture after exposure to 2.5, 10, and 20 μg cm^{-2} PET using Mitoprobe™ assay. One-way ANOVA followed by Dunnett's multiple comparisons test ($\alpha = 0.05$) showed no significant effect at 2.5 μg cm^{-2} ($p = 0.0730$), but significant reductions in the high-fluorescent population at 10 μg cm^{-2} ($p = 0.0020$) and 20 μg cm^{-2} ($p = 0.0040$), consistent with loss of mitochondrial membrane potential. Together, these findings link a real-world school exposure scenario to early PET-associated cellular responses in a lung barrier-relevant model.

Acknowledgements: São Paulo Research Foundation (FAPESP) grants 2022/03087-9, 2023/06768-0 and 2025/11879-0. **References**: [1]Zhang et al.; *Earth Sci Rev* **2020**, 103118.; [2]Ferraz et al.; *Chemosphere* **2024**, v. 369, p. 143886. [3] Villacorta et al.; *J. Hazard. Mater* **2022**, v. 439, p. 129593.

EES - D4 - P28
Optimising reaction efficiency with surfactants

Rachel Napier[1], Nikil Kapur[2], John Blacker[1], Hannah Hayes[3] , Bao Nguyen[1]
[1]School of Chemistry, University of Leeds, UK; [2]School of Mechanical Engineering, University of Leeds, UK; [3]Chemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, UK.

Modern organic chemistry relies heavily on petroleum-based organic solvents, creating significant environmental burdens. Surfactants in water can be utilised to replace organic solvents and facilitate greener routes to organic molecules.[1] While expensive designer surfactants, such as TPGS-750-M and PS-750-M, are principally used, inexpensive and commercially available surfactants can perform equally well, making a process economically viable for large–scale industrial applications. The ***surfactant_map***[2] is a data-driven tool developed within the Institute of Process Research and Development (iPRD) at the University of Leeds, to guide rational surfactant selection for any given reaction.

A major barrier to the broader adoption of surfactant-enabled reactions lies in reaction work-up/purification. The amphiphilic nature of surfactants makes their removal particularly challenging, often requiring large volumes of organic solvents during work-up, negating the sustainability benefits of these reactions. A coalescing separator is a depth filter made from meltblown media that utilises both surface and gravity forces to separate immiscible liquids.[3,4] Coalescing filters are effective at breaking strong emulsions, making them well suited for overcoming the challenges associated with surfactants at the work-up/purification stage. This work has demonstrated the successful application of a novel coalescing separator, developed within the iPRD, to effectively eliminate surfactant contamination for high-yielding surfactant-enabled S_NAr and amide coupling reactions, previously optimised using the ***surfactant_map.*** Furthermore, the coalescing separator can be integrated into a continuous platform, offering the potential for continuous surfactant-enabled synthesis with in-line extraction and surfactant recycling.

Overall, the implementation of the ***surfactant_map,*** continuous flow chemistry and coalescing separators to deliver cost-effective, high-yielding surfactant-enabled reactions free from surfactant contamination represents a significant step toward industrially relevant, low-waste aqueous reaction platforms.

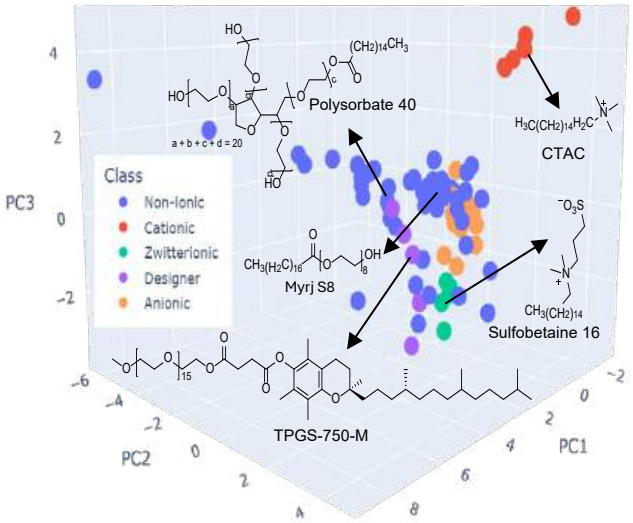

Fig. 1. The ***surfactant_map***.[2]

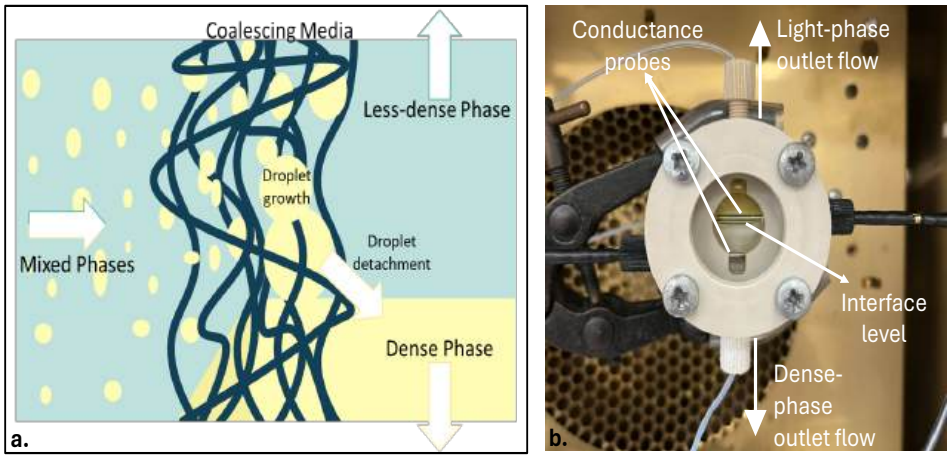

Fig. 2. **a.** Schematic of phase separation with a coalescing filter. **b.** Front-on view of the coalescing separator.

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EES - D4 - P29

Revealing the extraction and coordination behavior of novel cyclohexyl o-oxydiamides ligand toward Pu(IV) μ

Qi Chen, Taihong Yan, Tianchi Li, Yandong Sun, Ye Zhang, Xiao Ge.
China Institute of Atomic Energy

Plutonium is of strategic importance. The study of Pu selective separation from nuclear industry liquid waste is crucial for Pu recovery. The present study is based on the plutonium-selective specific ligand o-phenoxydiamide, the benzene ring in its structure was replaced by cyclohexane, and the new cyclohexyl o-oxydiamide (R-CAD) was predicted to have a spatial spin while maintaining a high charge density, will be involved in the coordination with Pu(IV) as a tetradentate ligand, and will facilitate for Pu(IV) extraction. The coordination behavior was further explored by slope analysis, Ultraviolet-Visible titration, and FT-IR analysis, which proved that R-CDAforms of 1:1 and 1:2 metal/ligand complexing with Pu(IV) through four hard oxygen (ether oxygen and carbonyl oxygen) in the structure, with the 1:2 complexes displaying higher stability. Density functional theory (DFT) calculations revealed that the carbonyl oxygen atom in the complex had a far greater affinity for Pu(IV) than did the ether oxygen atom. In addition, the 1:2 metal/ligand complex single-crystal structure formed by R-CDA with Pu(IV) has been discovered for the first time in a breakthrough manner, and the coordination form has been elucidated intuitively. On the other hand, it was confirmed that R-CDA has good acid and irradiation stability. The present study not only enriches the theoretical knowledge of the coordination chemistry of Pu(IV) but also offers fresh perspectives on the design of separation ligands for plutonium in the nuclear industry.

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EES - D4 - P30

Selective extraction of plutonium(IV) by novel diphenylpyridine diamide extractants

Yao Liu, Junli Wang, Wang Junli, Le Yuhang, Wang Hui, Wang Wentao, Li Baole, Ye Guoan, Yan Taihong
China Institute of Atomic Energy

Three novel diphenylpyridine diamide extractants, PPDA, PDBA and PMDA, were designed and synthesized for the selective extraction of Pu(IV) from complex nitric acid systems. Their extraction behavior was systematically investigated by solvent extraction experiments, spectroscopic titrations and density functional theory calculations. All three ligands exhibited excellent extraction ability toward Pu(IV) and high selectivity over competing actinides and fission products. In particular, they enabled effective separation of Pu(IV) from other tetravalent metal ions, which remains a major challenge in plutonium separation chemistry. Slope analysis and UV–Vis titration showed that the extracted complexes had a 1:1 metal-to-ligand stoichiometry. Thermodynamic studies indicated that the extraction process was spontaneous and exothermic under ambient conditions. The stability constants further confirmed the strong complexation ability of these ligands toward Pu(IV). DFT calculations revealed that the stronger Pu–O interaction, compared with other metal–oxygen bonds, plays a key role in the observed selectivity. In addition, the ligands showed good reusability and irradiation stability, maintaining their extraction performance after repeated cycles and gamma irradiation. These results demonstrate that the newly developed diphenylpyridine diamide ligands are promising candidates for the efficient and selective separation of Pu(IV) from complex systems.

Supported by basic support for stability of China Institute of Atomic Energy (BJ030261224901).

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EES - D4 - P31
A green and efficient aqueous LLPS platform for metal ion separation

Ruihan Yan, Wentao Wang*, Zhi Cao, Qi Chen, Taihong Yan*
Dept. of Radiochemistry, China Institute of Atomic Energy, China

The traditional aqueous-organic biphasic extraction for separating metal ions faces major challenges due to heavy reliance on volatile organic solvents and the resulting refractory radioactive waste. Aqueous liquid-liquid phase separation (LLPS) offers an alternative by forming a condensed separation phase directly in water, yet its research in metal ions separation is still limited. Here, we establish LLPS as a separation platform through two complementary modes: self-extracting and extractant-loaded. In the self-extracting mode, quaternary ammonium surfactants/HFIP condensed phase enables near-quantitative extraction of Au(III), Pt(IV), and Pd(II) under mild aqueous conditions. This mode also maintains selective Au(III) recovery from real PCB leachates at an extreme Cu/Au mass ratio of 4300:1, with an enrichment factor of 25. Moreover, using only 1 mM thiourea as the stripping reagent, the condensed phase sustains five extraction-stripping cycles with average extraction and stripping yields of 97.6% and 97.9%, respectively. In the extractant-loaded mode, an SDS/CTAB/HFIP condensed phase encapsulates commercial extractants to provide programmable radioactive-ion separation. In simulated high-level liquid waste, the extractant-loaded aqueous LLPS system achieved a U(VI) distribution ratio of 1.29×10^3, with separation factors exceeding 10^3 over coexisting lanthanides and alkaline-earth metal ions, demonstrating highly selective U(VI) partitioning. After stripping with 0.05 M EDTA, this system maintains extraction yields above 98% over five cycles, while the average stripping yield remained above 92%. Despite their distinct target chemistries, both modes follow the same design logic: LLPS forms a small and independent condensed phase in the original aqueous phase. Selective metal ions partitioning is governed by the synergistic effect of supramolecular interactions, particularly electrostatic and hydrophobic interactions, and metal-ligand coordination. Above all, these results show that aqueous LLPS is a tunable, green and efficient framework for selective metal-ion separation across distinct separation scenarios.

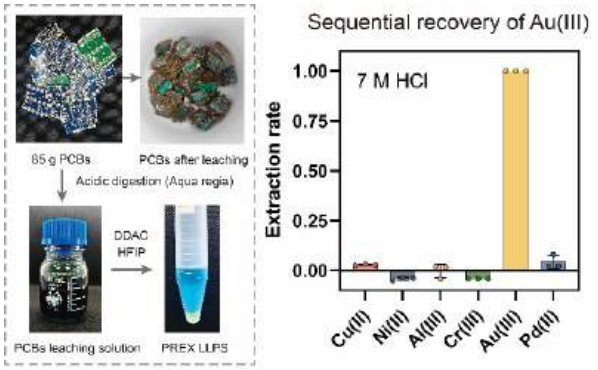

Fig. 1. Practical application for PMs separation from discarded mobile phone PCBs.

Fig. 2. Schematic of the extractant-loaded system (SCH-extraction system) formation process and generation mechanism.

The authors gratefully acknowledge the support from the Continuous-Support Basic Scientific Research Project (BJ030261224901, BJ030261224862).

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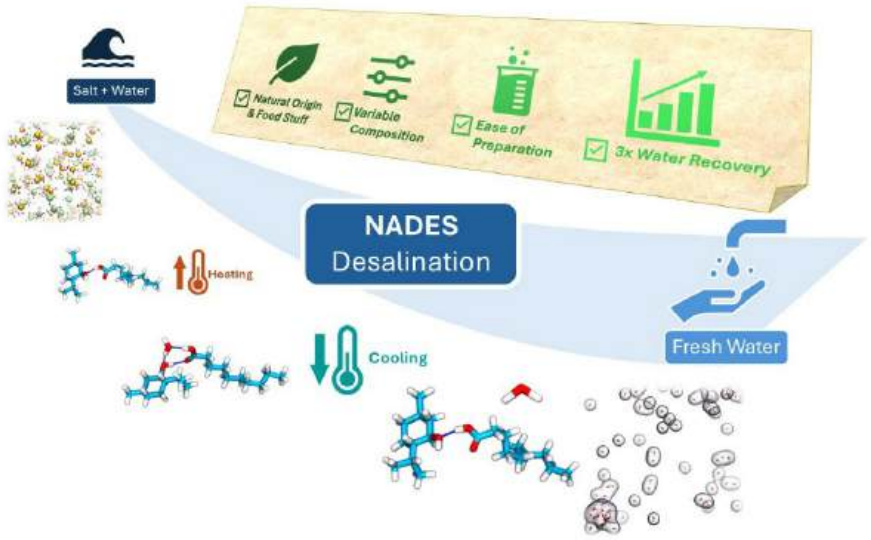
EES - D4 - P32
Green extractive desalination with designer green solvents for freshwater production

PingKeung Wong[1], LokWan Ng[1], Wei Han[1], Matthew Y. Lui[1]
[1]Hong Kong Baptist University, HKSAR

Extractive desalination represents an affordable, membrane-less approach to desalinate water, which can operate solely using low-temperature waste heat from industrial sources. It has been suggested as a viable alternative for producing freshwater from saline sources by employing long-chain carboxylic acids.[1] To enhance the freshwater yield, ionic liquids (ILs)[2-3] and amines[4] have been explored as replacements for carboxylic acids. Nevertheless, amines exhibit significant toxicity, and ILs frequently contain hazardous elements, particularly the bis(trifluoromethanesulfonyl)imide anion.
To balance high water recovery with a green and food-based solvent selection, we identified the most effective designer green solvent for extractive desalination, especially the hydrophobic natural deep eutectic solvent (NADESs). Initial findings show that these NADESs improve overall freshwater yield and salt rejection relative to their individual constituents. This enhancement occurs through the disruption of robust dimeric hydrogen bonds between solvent molecules, which otherwise impede water uptake, and by extending the duration of hydrogen bonds formed between the extractant and water. The resulting fresh water exhibits minimal salinity, complying with World Health Organization guidelines, and is suitable for direct consumption by humans and land animals—in contrast to earlier proposed extractants.



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EES - D4 - P33

MXene-promoted Ni-based bimetallic catalysts on CeO_2–ZrO_2 for efficient hydrogen production via steam methane reforming

Shahid Ali[1,*], Abdul Zeeshan Khan[1], Muhammad Mansha[1], Safyan Akram Khan[1]
[1]*Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum and Minerals, Saudi Arabia*
*Corresponding Author Email: s.ali@kfupm.edu.sa

Hydrogen is widely recognized as a key energy carrier in the global transition toward low-carbon and sustainable energy systems, with applications across industrial processes, power generation, and transportation. Among available technologies, steam methane reforming (SMR) remains the most cost-effective and industrially established route for large-scale hydrogen production. However, conventional SMR catalysts are limited by sintering, coke formation, thermal instability, and reduced activity at lower operating temperatures, highlighting the need for advanced and durable catalyst systems. Herein, we report the development of multifunctional SMR catalysts based on MXene-promoted Ni–Co bimetallic nanoparticles supported on CeO_2–ZrO_2. The optimized catalyst composition consists of Ni, Co, and MXenes dispersed on CeO_2–ZrO_2 support. This integrated design combines the high oxygen storage capacity and thermal stability of the CeO_2–ZrO_2 support with the synergistic effects of Ni–Co bimetallic active sites and MXene promotion. This results in enhanced metal dispersion, strengthened metal–support interactions, and improved resistance to sintering and carbon deposition. The catalysts were comprehensively characterized using X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), dynamic light scattering (DLS), thermogravimetric analysis (TGA), and Brunauer–Emmett–Teller (BET) surface area analysis. Structural characterization confirmed a high surface area and uniform distribution of active sites. Catalytic performance evaluation demonstrated high methane conversion and enhanced hydrogen yields (>90%) under SMR conditions. Overall, this multifunctional catalyst strategy effectively addresses the limitations of conventional SMR catalysts, offering a promising pathway toward more efficient and sustainable hydrogen production.

Acknowledgement: The authors acknowledge financial support provided by King Fahd University of Petroleum and Minerals (KFUPM), Kingdom of Saudi Arabia, for this research under the IRC-HTCM Project (INHT2525).

EES - D4 - P34
Natural Algerian diatomite as a low-cost adsorbent for Bezacryl yellow dye removal

Daouia Ingrachen-Brahmi[1], Hocine Ouadi[1], Sylia Azoug[1]
[1]University of Bejaia, Faculty of Exact Sciences, Laboratory of Materials Technology and Process Engineering (LTMGP), Algeria

Water pollution by synthetic dyes is a significant environmental issue in Algeria. This study evaluates Algerian diatomite known Kieselguhrs as a low-cost and sustainable adsorbent for the removal of Bezacryl Yellow (BY) from aqueous solutions. Diatomite (D) is characterized by different physical-chemical methods (X-ray diffraction, scanning electron microscopy, Fourier transform infrared and Thermogravimetric analysis (TGA). The adsorbent exhibits a specific surface area of 163 $m^2.g^{-1}$, determined by the Sears method[1,2]. Batch adsorption experiments were conducted under various conditions of pH, adsorbent dosage, dye concentration, contact time, and temperature. Adsorption was found to be strongly favored in highly alkaline media at pH =12, B Yremoval rate increases as pH increases. Adsorption equilibrium is reached after 20 mins of contact time. Kinetic data were best described by the pseudo-second-order (PSO) model, while equilibrium results followed the Temkin isotherm, indicating uniform adsorption energy distribution. A maximum adsorption capacity of 212 mg.g-1 was obtained. Thermodynamic analysis revealed a negative enthalpy change ($\Delta H° = -9.451$ kJ mol^{-1}), confirming an exothermic process favored at lower temperatures. These results demonstrate that Algerian diatomite is an efficient, eco-friendly, and economically viable adsorbent for the removal of Bezacryl Yellow from contaminated water.

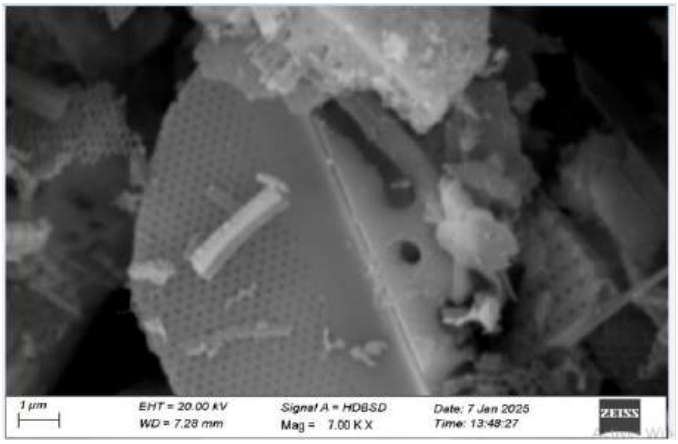

Fig. 1. SEM micrograph of raw diatomite powder at scale bar of 1 µm.

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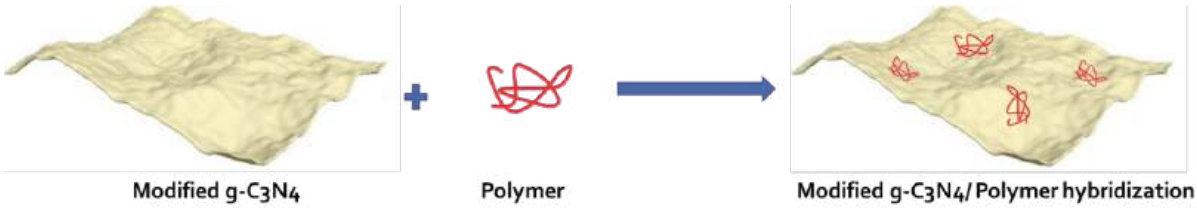
EES - D4 - P35

Enhanced photocatalytic hydrogen evolution via broad visible-light harvesting in g-C_3N_4/polymer heterostructures

Mohamed Hammad Elsayed[1]

[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum & Minerals, Saudi Arabia

Graphitic carbon nitride (g-C_3N_4) is a widely investigated metal-free polymeric semiconductor for photocatalytic hydrogen evolution and CO_2 reduction because of its suitable band gap (2.7 eV), visible-light activity, thermal stability, low cost, and non-toxic nature[1]. However, its practical photocatalytic performance remains limited by rapid charge-carrier recombination and weak light absorption beyond 460 nm. To overcome these drawbacks, heterostructured photocatalysts based on g-C_3N_4 and organic conjugated polymers have attracted growing attention, owing to their tunable electronic structures and improved charge-transfer properties. In this work, modified g-C_3N_4 was hybridized with a conjugated polymer possessing broad visible-light absorption and good solubility to strengthen interfacial interactions and extend optical absorption, thereby enhancing photocatalytic activity. Among the prepared g-C_3N_4/polymer heterostructures, the g-C_3N_4/PFTBTA photocatalyst exhibited the best hydrogen evolution rate of 833.81 umol h^{-1} in the presence of ascorbic acid as a sacrificial agent. Notably, the g-C_3N_4/PFTBTA heterostructure delivered an outstanding apparent quantum yield (AQY) of 84% at 500 nm, outperforming all comparable materials reported to date.



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EES - D4 - P36

Energy-efficient and sustainable water desalination using flow electrode deionization with enhanced charge and ion transfer

Abdullah Alsultan[1]
[1]Jubail Industrial College, Saudi Arabia

The increasing demand for freshwater requires the development of energy-efficient and sustainable desalination technologies. Flow electrode deionization (FEDI) is a promising electrochemical approach for continuous desalination; however, its performance is often limited by inefficient charge transfer and restricted ion transport within the system.

In this study, an enhanced FEDI system was developed by integrating a three-dimensional carbon foam current collector with ion exchange resin to enhance overall electrochemical performance. The carbon foam provides a highly conductive porous structure that enhances electron transfer, while the ion exchange resin facilitates ion migration by forming conductive pathways and reducing mass transfer resistance.

The optimized system achieved an average salt removal rate of 845 $\mu g \cdot cm^{-2} \cdot min^{-1}$ with a low electrical energy consumption of 1.64 $J \cdot mg^{-1}$, demonstrating energy-efficient desalination while maintaining competitive removal performance. This performance is attributed to reduced internal resistance and more efficient utilization of electrical charge.

These results demonstrate a practical strategy for improving electrochemical desalination systems and support the development of scalable, energy-efficient technologies for sustainable water treatment.

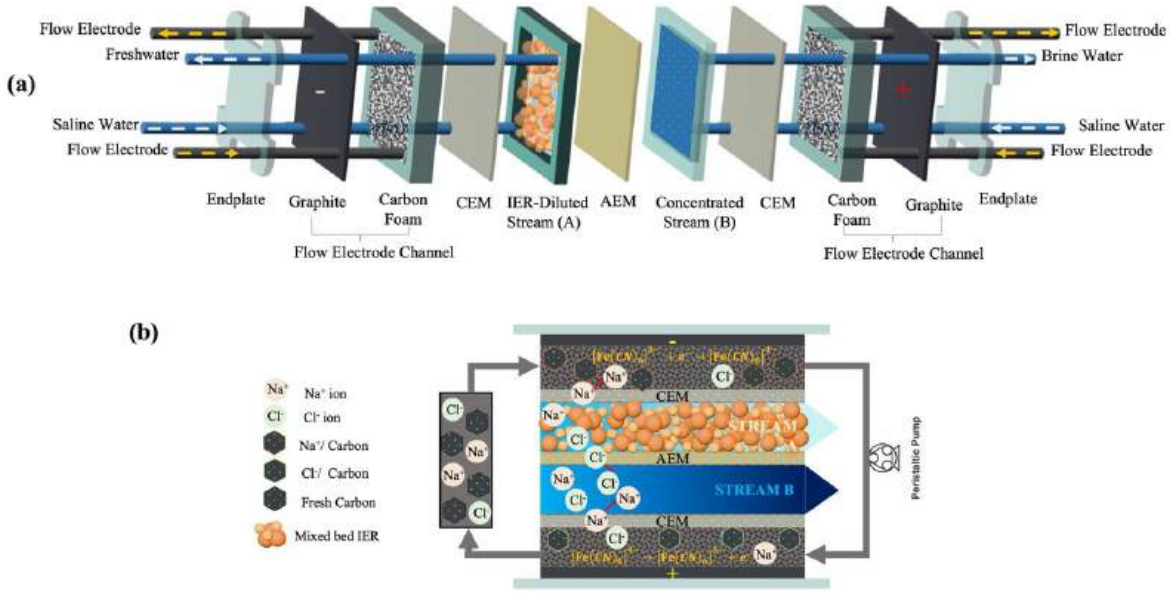

Fig. 3. (a) Schematic illustration of the flow electrode deionization (FEDI) system and (b) experimental setup used for continuous desalination.

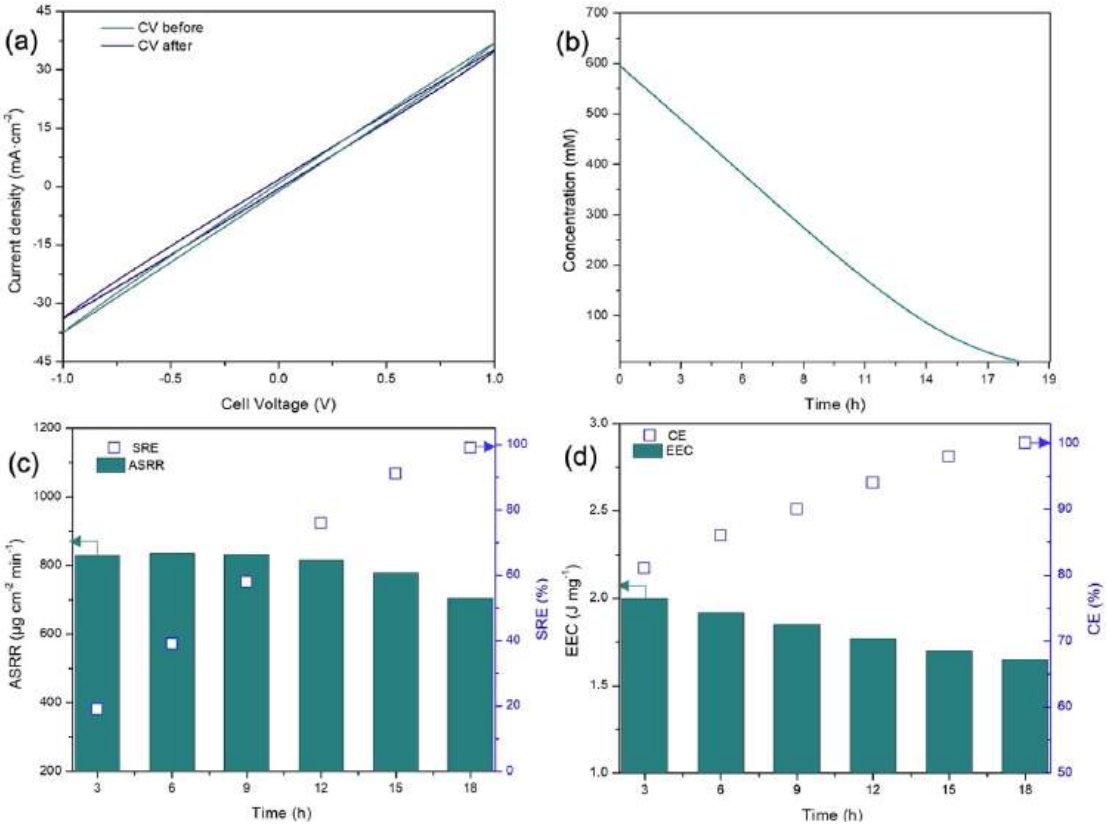

Fig. 2. Electrochemical and desalination performance of the optimized FEDI system: (a) cyclic voltammetry response, (b) salt concentration profile, and (c–d) key performance metrics including salt removal rate and energy consumption.

EES - D4 - P37
Graphene quantum dot-based nanostructured electrodes for advanced sodium ion batteries

Grainne Gilleece[1], Dagou Zeze[1], Natasha Shirshova[1], Ensieh Hosseini[1]
[1]Durham University, Dept. of Engineering, Lower Mountjoy

Tungsten disulfide (WS_2) is a layered transition metal dichalcogenide (TMD) with rich redox chemistry and a high theoretical capacity. It is therefore a promising anode material for sodium-ion batteries (SIBs). However, WS_2 suffers from low conductivity, structural instability upon cycling and limited sodium ion diffusion kinetics. The addition of nitrogen-doped graphene quantum dots (N-GQDs) to WS_2 can mitigate these issues. GQDs provide further active sites, an increased surface area, and can act as a structure regulator. Furthermore, the nitrogen doping of the GQDs provides a greater number of ion diffusion channels and leads to a higher charge carrier density.

N-GQDs with highly controllable bandgaps were first synthesised. The edge shapes and size of the nanoparticles were selected, alongside the battery electrolyte pH, to provide the most beneficial properties for SIBs. Self-assembled low crystallinity tungsten disulfide nanosheets with embedded N-GQDs were grown on the surface of nickel foam via electrodeposition, creating a binder-free anode. SEM images confirmed the presence of the nanosheets, while EDX, UV Vis and Raman confirmed their composition. XRD and SAED data demonstrated that the interlayer spacing of the WS_2 was widened by 0.1 nm (from 0.62 to 0.72 nm) upon N-GQD addition.

The widened interlayer spacing facilitates sodium-ion intercalation and conversion recations. The N-GQD/ WS_2 electrode has a specific capacity of 311 mAh/ g at 1 A/ g, compared to 206 mAh/ g for the electrode without N-GQDs integrated.

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Posters

Innovative Materials (IM)

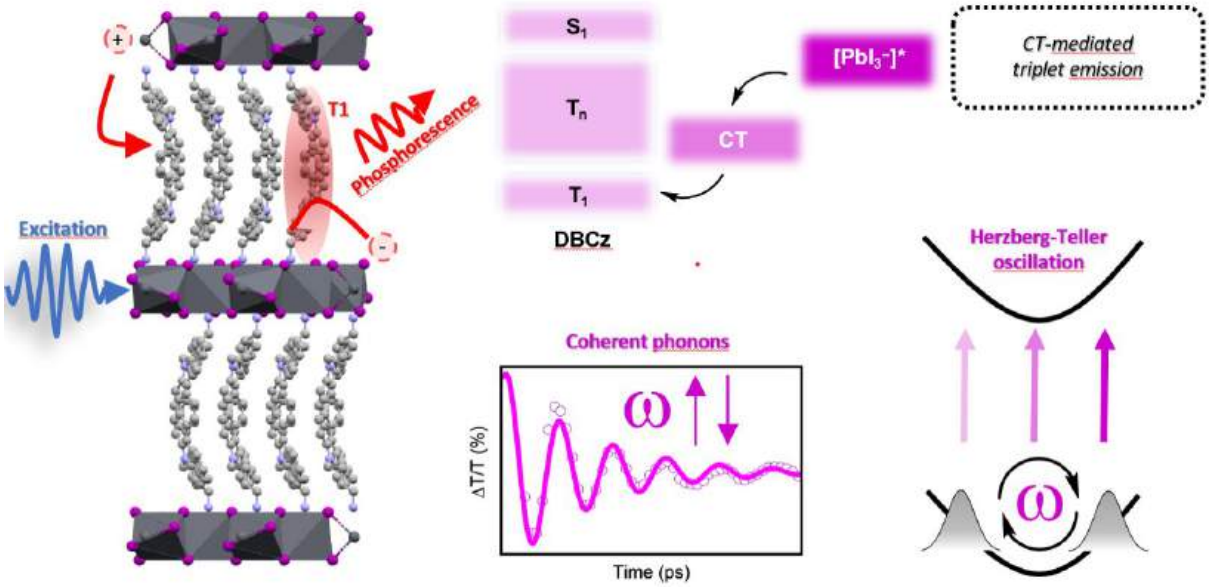
IM - D1 - P04

Ultrafast charge transfer and coherent phonons in electroactive organic cation-templated low-dimensional perovskite analogues

Ilan Devroey[1,2†], Yorrick Boeije[3,4†], Peter Banks[5], Claudio Quarti[5], Paola La Magna[6], Aleksandra Ciesielska[1,2], Laurence Lutsen[2,7], Elien Derveaux[7,8], Peter Adriaensens[7,8], Kristof Van Hecke[6], David Beljonne[5], Samuel D. Stranks*[3,4], Wouter T.M. Van Gompel*[1,2,7]

[1]Hasselt University, Institute for Materials Research (imo-imomec), Hybrid Materials Design (HyMaD), Hasselt, Belgium; [2]Energyville, imo-imomec, Genk, Belgium; [3]University of Cambridge, Dept. of Chemical Engineering and Biotechnology, Cambridge, UK; [4]University of Cambridge, Dept. of Physics, Cavendish Laboratory, Cambridge, UK; [5]University of Mons, Laboratory for Chemistry of Novel Materials, Materials Research Institute, Mons, Belgium; [6]Ghent University, Dept. of Chemistry, XStruct, Krijgslaan, Ghent, Belgium; [7]imec, imo-imomec, Diepenbeek, Belgium; [8]Hasselt University, Institute for Materials Research (imo-imomec), Applied and Analytical Chemistry, NMR group, Hasselt, Belgium

Hybrid organic-inorganic perovskites (HOIPs) have emerged as promising materials for optoelectronic applications, yet gaining control over their structural and electronic tunability remains a key challenge. In this study, we introduce 7H-dibenzo[*c*,*g*]carbazole (DBCz) as a novel electroactive organic cation that enables the formation of two distinct low-dimensional hybrid metal halides: a conventional 2D perovskite structure, $(DBCz)_2PbI_4$, and a previously unreported layered perovskite analogue structure with edge-sharing octahedra, $DBCzPbI_3$. The edge-sharing phase represents a new structural motif within the hybrid metal halide family. Both materials exhibit a type-II band alignment, facilitating ultrafast photoinduced hole transfer from the inorganic to the organic layer. Using transient absorption spectroscopy, we identify the formation of DBCz-based hole polarons in both phases, and uniquely observe the charge-transfer-induced formation of triplet states and room-temperature coherent phonons for the perovskite analogue phase. These findings highlight the role of molecular design in controlling excited-state dynamics and exciton–lattice interactions in hybrid metal halides.



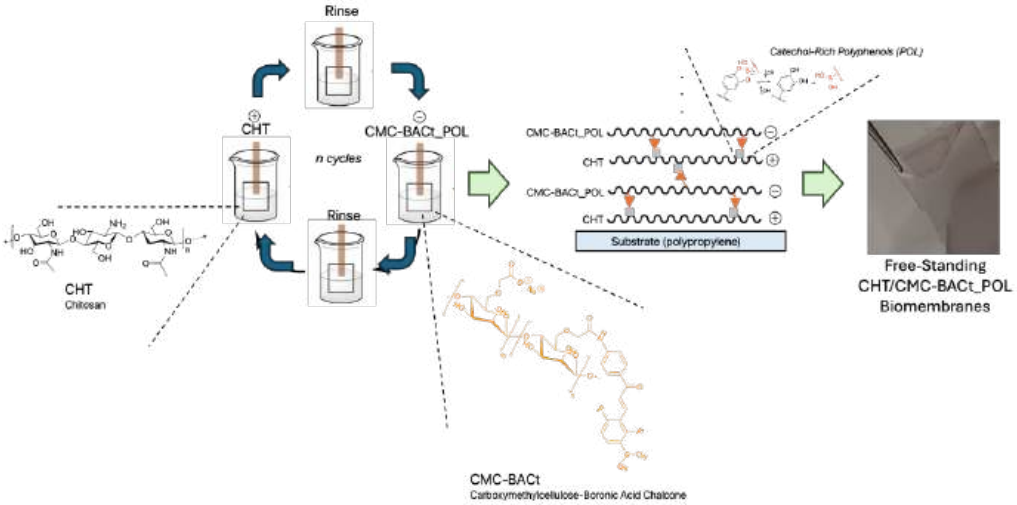
I. D. acknowledges the Research Foundation – Flanders (FWO) for the funding of their FWO strategic basic research PhD grant (1S31325N).

IM - D1 - P05

Layer-by-layer supramolecular assembly of boronic acid chalcone-containing biomembranes for pH-controlled complexation of catechol-rich polyphenols

Luís Cruz, Mariana Cunha, Victor de Freitas
REQUIMTE/LAQV, Dept. of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Portugal

The fabrication of functional and smart (stimulus-responsive) biomaterials has been an emerging area for a wide range of applications from food science, biomedicine, and materials engineering. Particularly, the design of materials containing boronate-catechol interactions is a versatile tool in molecular recognition, sensing, and drug delivery due to their ability to be triggered by specific analytes or by alterations of physicochemical parameters such as pH.
In this work, the fabrication of sustainable and free-standing multilayered membranes using carboxymethyl-cellulose-modified boronic acid chalcone receptor (CMC-BACt), chitosan (CHT) and catechol-rich polyphenols (POL) was pursued. To this purpose, the boronic acid-chalcone receptor (BACt) was first synthesized through a basic-catalyzed aldol condensation and further used for the functionalization of carboxymethylcellulose (CMC) through carbodiimide coupling chemistry. Afterwards, the positively charged CHT solution was combined with the negatively charged CMC-BACt solution (containing POL) to fabricate multilayered biomembranes through electrostatic-driven interactions using Layer-by-Layer (LbL) supramolecular assembly methodology (Scheme 1).[1] The quantification of POL content within the biomembranes was quantified by HPLC, and their releasing kinetic profiles was studied in a pH-regulated manner. This work provides valuable insights into the binding affinity of structurally diverse catechol moieties within the polyphenol framework, offering a deeper understanding of dynamic boronate-catechol complexation, envisaging advanced applications in active and sensing food packaging materials.



Scheme 1. Fabrication of multi-layered CHT/CMC-BACt_POL biomembranes through LbL technology.

Acknowledgments: Luís Cruz gratefully acknowledges FCT for the research contract funded through the Individual Call to Scientific Employment Stimulus with reference 2023.07923.CEECIND/CP2842/CT0001. Mariana Cunha acknowledges FCT for the PhD grant (2024.01342.BD).

Funding: This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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IM - D1 - P06
Ti-based core-shell shaping for Ac-225/Bi-213 separation

Thomas Staes[1,2,3], Vera Meynen[2,3], Steven Mullens[2], Janne Gys[1], Thomas Cardinaels[2], Bart Geboes[1]
[1]Belgian Nuclear Research Centre, SCK CEN, Mol, Belgium; [2]Flemish Institute for Technological Research, VITO, Mol, Belgium; [3]University of Antwerp, Antwerp, Belgium

Cancer remains one of the leading causes of death worldwide, requiring innovative methods for its treatment such as **targeted alpha therapy with ^{213}Bi-based radiopharmaceuticals**. Alpha radiation is especially promising as it enables maximum destruction of malignant cells while minimizing cytotoxicity on the surrounding healthy tissue. However, **current challenges in separating the radioactive ^{213}Bi** from the mother ^{225}Ac isotope **prevent more widespread use** in a clinical environment despite the promising results. Therefore, the development of an **innovative new sorbent material** with a long operational lifetime (~10 days), **shaped to enable** the required **fast (de)-sorption kinetics** (≥80% ^{213}Bi yield in 2 mL eluate), is needed. Moreover, the harsh separation conditions—exposure to highly acidic medium (< pH 3) and high radiolytic dosages (~4 GBq)—limit the number of materials qualified for this application. Although inorganic support materials show potential, they need to be shaped to an appropriate macroscopic architecture which allows sufficiently fast (de)-sorption kinetics. The aim of this project is to develop a **micron-sized core-shell type stationary phase** consisting of a **Ti-support with tuned surface porosity** that promote the desired fast (de)-sorption kinetics, while adjusting chemical composition and structural features **to provide optimal separation performance** (selectivity and yield) in combination **with radiation and acid stability**.

This work is supported by the Research Foundation Flanders (FWO) through project 1S45925N-7021.

IM - D1 - P07

Unraveling competing reactions in the synthesis of renewable α-methylene-γ-valerolactone

Féline De Meester[1], Pieter Billen[1], Christophe M.L. Vande Velde[1] , Yoshi W. Marien[1,2]

[1]Intelligence in Processes, Advanced Catalysts and Solvents (iPRACS) Faculty of Applied Engineering, University of Antwerp, Antwerp, Belgium; [2]Laboratory for Chemical Technology (LCT), Ghent University, Zwijnaarde, Belgium

α-methylene-γ-valerolactone (MGVL) is a renewable monomer that shows structural resemblance to methyl methacrylate (MMA), making it a promising candidate for high performance polymers. Polymerization studies indicate that poly(MGVL) exhibits superior properties.[1-4] However, the synthesis of MGVL remains challenging. Existing routes either rely on formalin gas or on thermal cracking of paraformaldehyde. The latter approach is more practical but suffers from low selectivity.[5] Generally the synthesis proceeds via Claisen-condensation. However, the identity of side-products are poorly understood.

The temperature- and time-dependence of MGVL synthesis was investigated. Reaction performance was evaluated as a function of the selectivity towards the desired product and quantified by GC-FID. Time-dependent studies revealed that a minimum reaction time of 16 hours is required to observe even trace amounts of monomer formation. Across a series of experiments (16-24 hours), monomer selectivity reached an optimum at 20 hours. Beyond this point, selectivity decreased. Monomer formation is enhanced by temperature but also increase side-product formation.

To elucidate the underlying chemistry, reaction mixtures will be fractionated via column chromatography, followed by 1H-NMR to identify major side-products and competing pathways. GC-MS data indicate that one possible side-product may arise from spontaneous dimerization. Together, these results provide insights into how reaction conditions influence both desired and undesired transformations, informing strategies for improved MGVL synthesis using paraformaldehyde.

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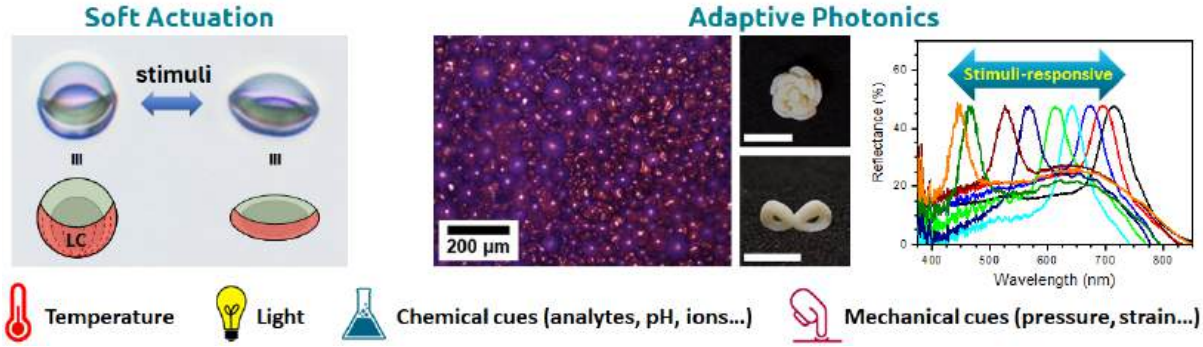
IM - D1 - P08
Liquid crystal emulsions as multifunctional platforms for soft actuation and adaptive photonics

Almudena Terrel, Mauricio Vera-Arévalo, Alberto Concellón
Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain

Liquid crystal (LC) emulsions have emerged as highly versatile soft matter systems in which interfacial geometry and molecular order can be precisely engineered to access a wide range of adaptive functionalities.[1] By combining the dynamic morphologies of complex emulsions with the anisotropic ordering of LCs, these systems provide a powerful platform for creating responsive microstructured materials with coupled mechanical and optical properties.[2,3]
In this presentation, we show how LC emulsions can be engineered into multifunctional microstructured materials by leveraging their programmable morphology and internal LC order. LC microparticles are fabricated via photo-initiated radical polymerization of LC emulsions, yielding single- and multiphase architectures with controlled interfacial organization. The resulting particles undergo reversible, anisotropic shape transformations in response to external stimuli such as temperature, light, or solvent exposure. These deformations enable soft actuation at the microscale and can be directly exploited to create adaptive microlenses with thermally tunable focal plane and magnification.
Moreover, LC emulsions can be translated into additively manufactured architectures by functioning as printable, multifunctional inks.[4] Using polymerizable LC emulsion droplets in 3D printing, we fabricate complex three-dimensional objects that preserve the internal LC ordering of the precursor droplets. Incorporation of chiral nematic LCs into these emulsion-based architectures gives rise to intrinsic structural color and selective light reflection arising from the helical LC organization, producing vivid, monochromatic and angle-independent color microstructures. Importantly, the reflected color and optical response can be dynamically tuned by external stimuli such as temperature, light, the chemical environment (e.g., pH or specific cations), and mechanical deformation, enabling color-adaptive and reconfigurable photonic microstructures.
Together, these results highlight LC emulsions as a general and modular platform with strong potential to bridge fundamental science and applied technology.



This work was financially supported by projects PID2023-146811NA-I00 and RYC2021-031154-I, funded by MICIU/AEI/10.13039/501100011033 and “ERDF A way of making Europe”; Fundación Ramón Areces (project CIVP22A7601); and Gobierno de Aragón–FSE (research group E47_23R). MVA thanks MICIU/AEI for his PhD grant (FPU24/01406).

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IM - D1 - P09

RENOVATE-PU: Recycle the non-recyclable by valorizing industrial chemical recycling techniques for polyurethane

Zoë De Herdt[1], Pieter Billen[1], Christophe M.L. Vande Velde[1]
[1]*University of Antwerp, Belgium*

Polyurethanes (PUs) are versatile polymers produced via the polyaddition of polyols and diisocyanates, enabling applications from flexible and rigid foams to elastomers and fibers. Recycling remains particularly challenging for elastomers and fibers due to their high formulation complexity, including broad variation in polyols (polyether, polyester and specialty polyols). They are also frequently combined with other polymers, such as polyester in synthetic leather, which increases heterogeneity in post-consumer waste streams.
Given the small volumes and high compositional variability of these materials, developing dedicated recycling technologies or new infrastructure is economically unfeasible. Therefore, this work investigates whether the same glycolysis technology currently developed for flexible-foam recycling, a batch depolymerization process operated at 200 °C with excess ethylene glycol for 4 h, can be applied to these more complex PU waste streams. Depolymerization is followed by liquid–liquid extraction yielding a polyol-rich phase and an aromatic fraction. Target purities are <1000 ppm aromatics in the polyol-rich phase (REACH-compliant) and >99% purity in the aromatic fraction, enabling further valorization, including as feedstock for non-isocyanate polyurethanes.
This study shows that applying this technology to diverse PU waste streams is feasible, provided that appropriate pre-sorting procedures are implemented and, where necessary, minor batch modifications are introduced. Early results reveal that certain polyols and specific PU/polymer combinations can hinder depolymerization and phase separation, reducing recyclate quality. Identifying these limiting material characteristics enables practical sorting guidelines, supports long-term design-for-recycling strategies, and informs emerging regulatory frameworks, where difficult-to-recycle combinations may incur higher fees to incentivize more circular product design.

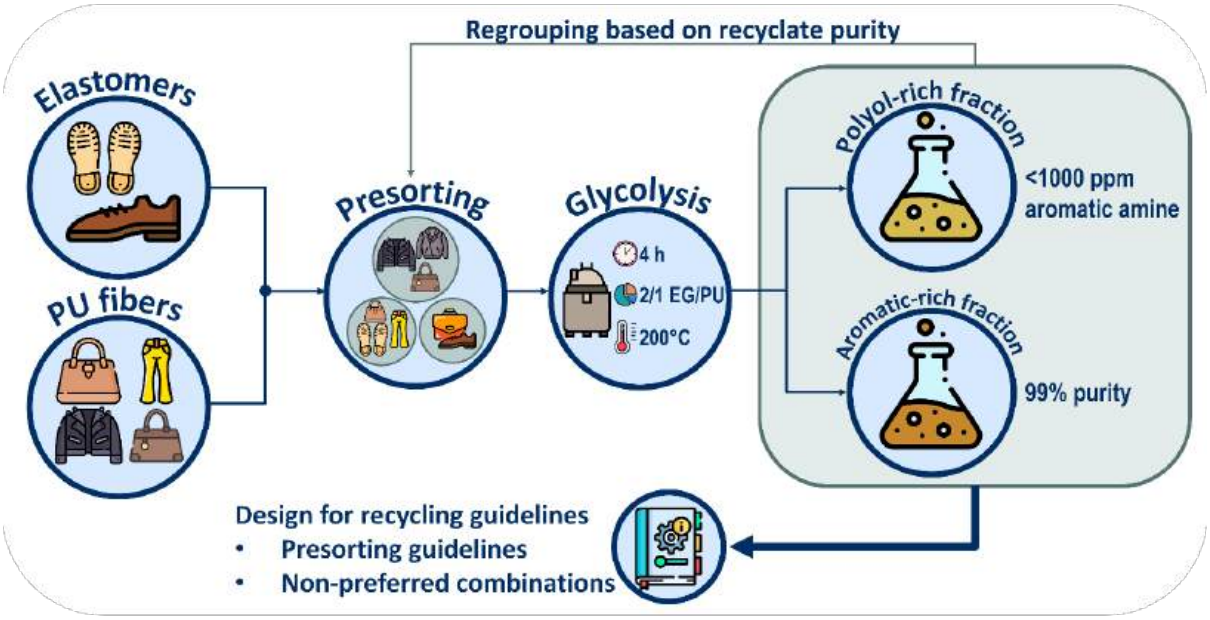

Fig. 1. Applicability of flexible-foam glycolysis to diverse and complex PU waste streams

IM - D1 - P10
Synthesis of phosphorus-sulfur containing Schiff base by Kabachnik-Fields reaction

Tzu Hsuan Chiang[1*], I-Chia Yang[1]
[1]Graduate College of Sustainability and Green Energy, National Central University, Taiwan

Phosphorus-containing Schiff bases have been widely applied as flame retardants [1] and as co-curing agents in wood surface coatings [2]. The imine (–HC=N–) functional group is known to form dynamically reversible intermolecular linkages even at room temperature without the need for external catalysts. In this study, a phosphorus–sulfur–containing Schiff base was synthesized via the Kabachnik–Fields reaction. Specifically, 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide (DOPO) was reacted with a mixture of thiodiacetic acid (TDA) and tetraethylenepentamine (TAPA) in anhydrous ethanol. The reaction mixture was heated to 85 °C under continuous stirring for 12 h. This synthesis route represents a green process, as it avoids the use of toxic solvents. Moreover, owing to the synergistic interaction among phosphorus, sulfur, and nitrogen species derived from DOPO and the sulfur-containing Schiff base structure, the resulting material exhibits a reduced OER overpotential during alkaline water electrolysis. These results highlight the beneficial role of P–S–N synergy in enhancing electrocatalytic activity.

Acknowledgements: This work was supported by the National Science and Technology Council, Taiwan, NSTC 113-2221-E-008-118-MY3.

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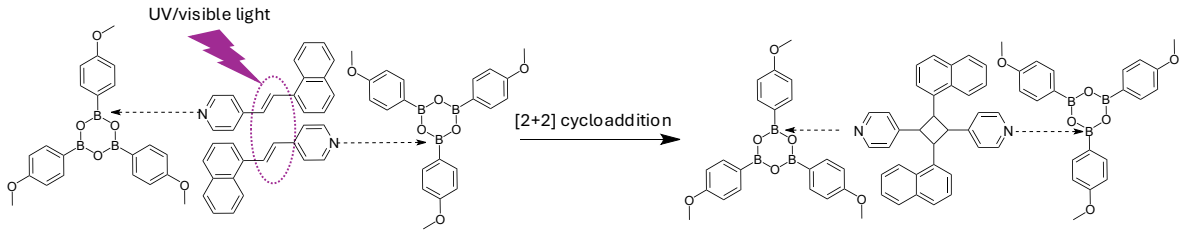
IM - D1 - P11
Structural mapping of photosalient B←N molecular crystals featuring intermediary dimer clusters

Wannes De Turck, Subhrajyoti Bhandary, Javed Pathan, Kristof Van Hecke
Ghent University, Belgium

Molecular crystals able to exert mechanical changes in response to external stimuli (light, heat, …) are promising smart materials for a variety of applications such as microscale actuators.[1,2] Photosalient crystals, or crystals that undergo abrupt mechanical motions under the influence of light, have been of particular interest. Molecular co-crystals composed of 4-(1-naphthylvinyl)pyridine with *para*-methoxytriphenylboroxine exhibit photosalient behaviour resulting from the formation of cyclobutane rings via a topochemical [2+2] cycloaddition reaction, upon exposure to UV, visible, or sunlight. Although similar processes have been previously discussed in literature,[3–5] the focus has been on understanding the intermolecular interactions at the level of individual olefin dimers. As such, a more holistic model has been lacking.
To resolve this, the transition from unreacted to fully converted crystals is followed and intermediaries, consisting of partially reacted crystals, isolated. Structural analysis of these intermediaries using single-crystal X-ray diffraction shows that the reaction between two olefins of a single dimer impacts the reactivity of the surrounding dimers. This effect is not limited to the first occurrence of a reacting dimer but continuous as the reaction spreads through a total of six dimers forming a cluster.



[2+2] cycloaddition reaction occurring between an olefin dimer under the influence of light with the formation of a cyclobutane bond as a result.

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IM - D1 - P12

Development of radiation-stable and selective sorbent materials for direct ^{213}Bi generators

Jasper Mampaey[1,2,3], Hilde Lenaerts[3], Vera Meynen[1], Steven Mullens[2], Thomas Cardinaels[2], Bart Geboes[3]
[1]University of Antwerp, Laboratory of Adsorption and Catalysis (LADCA), Belgium; [2]Flemish Institute for Technological Research (VITO), Belgium; [3]Belgian Nuclear Research Centre (SCK CEN), Belgium

Developing effective cancer treatment strategies remains a global challenge. Targeted alpha therapy (TAT) with ^{213}Bi as alpha emitter has emerged as a promising approach, offering cytotoxic effects on cancer cells while minimizing damage to healthy tissue. However, ^{213}Bi production is limited due to the lack of sorbent materials that are both selective and resistant to acidic environments and radiation, hindering efficient separation of ^{213}Bi from its parent ^{225}Ac. Given the urgent need for novel ^{225}Ac/^{213}Bi separation systems, known as ^{213}Bi generators, the potential of phosphate-modified titania as a sorbent material for their development is investigated. The synthesized materials were characterized by various techniques, such as zeta potential analysis, DRIFT spectroscopy, argon sorption and ^{31}P NMR, while batch sorption tests were conducted with La^{3+} (non-radioactive surrogate for ^{225}Ac) and Bi^{3+} to evaluate the sorption behaviour. Furthermore, the acidic and radiolytic stability of the phosphate-modified titania was evaluated by exposure to nitric acid and by irradiation with a ^{60}Co gamma source, respectively. The results showed that titania exhibited a high and selective Bi^{3+} uptake at low pH, regardless of the modification degree. La^{3+} removal, on the other hand, only reached similar levels to Bi^{3+} at pH ≥ 3 and with a sufficient degree of surface phosphate groups. Desorption experiments demonstrated efficient Bi^{3+} elution from the sorbent, although selectivity was limited due to substantial co-elution of La^{3+}. With respect to stability, titania showed high resistance to acidic degradation, but the leaching of phosphate surface groups did diminish sorption efficiency. Finally, exposure to gamma irradiation up to 5 MGy doses revealed an excellent radiolytic stability. In conclusion, this study demonstrates that, although modified titania needs further optimization before it could be applied in direct ^{213}Bi generators, unmodified titania could be envisaged as a highly promising sorbent for inverse ^{213}Bi generators.

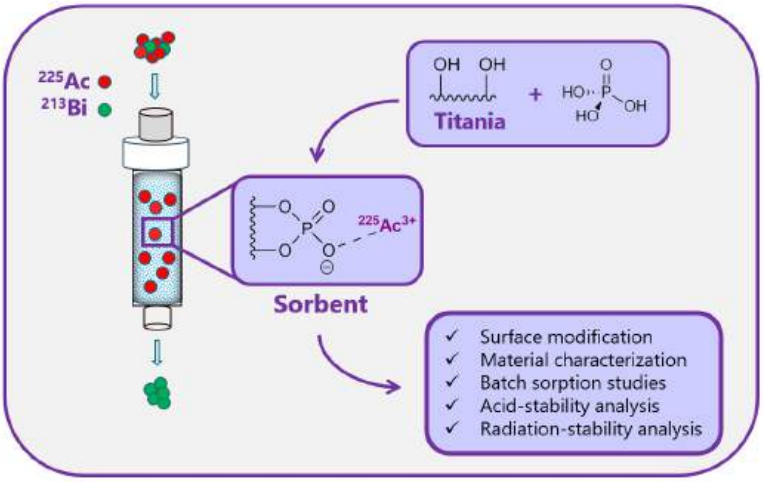

Fig. 2. Visual representation of research

IM - D1 - P13
Self-assembled polymer heterojunctions for solar to hydrogen

Corentin Pochet, Catherine Aitchison
Laboratory of Organic Electronics, ITN, Linköping University, Sweden

The conversion of solar energy to produce hydrogen through water splitting has the potential to be commercially viable if an efficiency of 10% can be reached.[1] Photocatalytic approaches typically use visible light absorbing semiconductors suspended as particles in water. However, these materials are expensive and require complex and energy intensive fabrication that is difficult to scale.
In contrast, ***organic conjugated polymer semiconductors*** are made up of cheap easily modifiable aromatic units with huge combinatorial flexibility and can produce hydrogen across much of the solar spectrum with quantum yields of up to 10% at 800 nm.[2] However, most reported systems only catalyse the hydrogen evolution half-reaction under sacrificial conditions.[3]
For overall water splitting, one challenge is overcoming the high exciton binding energies of organic semiconductors and generating the long-lived polarons, as water oxidation occurs with a longer timescale than hydrogen evolution. One of the most successful strategies is to use a ***donor-acceptor (D-A) heterojunction*** that interfaces a p-type and n-type semiconductor with offset energy levels to drive charge separation (Figure 1).[4]
Organic materials with more controllable secondary structures are also becoming of interest as highly ordered structures promote high activity toward proton reduction. This efficiency is thought to be the result of favoured energy transfer between the π-stacked sheets of these structures.[5,6] To enhance the charge transport properties of organic conjugated polymer semiconductors, ***crystallization-driven self-assembly (CDSA)*** stands as a powerful method as it generates organised and π-stacked nanofibers with promising optoelectronics properties.[7]
To promote efficient photocatalytic water splitting, we propose to incorporate ***D-A heterojunctions into nanofibers formed by CDSA*** (Figure 1). Our approach will enable a new class of heterojunction photocatalysts with optimised domain blocks for efficient charge separation and highly ordered packing for improved charge transfer to catalytic sites.

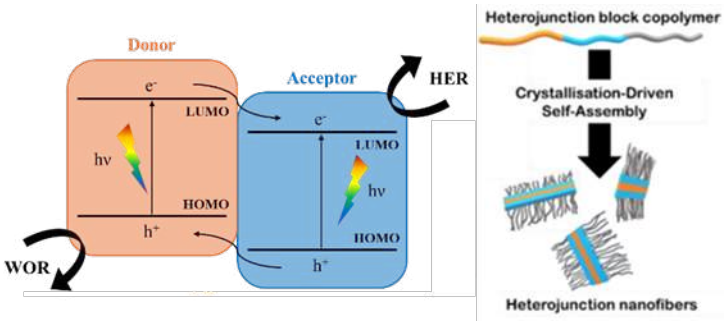

Fig. 3. Schematic of D-A heterojunctions and CDSA of nanofibers.

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IM - D1 - P14

Stability enhancement of polyetherimide under harsh space conditions via covalently bound self-passivating silica layers

Placido Mineo[1,2], Lidia Mezzina[1], Prospero Savoca[1], Maria Elisabetta Palumbo[3], Carlotta Scirè[3], Riccardo Giovanni Urso[3], Giuseppe Antonio Baratta[3], Anna Lucia Pellegrino[3], Laura Barone[1,3] and Angelo Nicosia[1]
[1]Dept. of Chemical Sciences, University of Catania, Italy; [2]Institute for Chemical and Physical Processes, National Research Council (IPCF-CNR), Messina, Italy; [3]INAF—Osservatorio Astrofisico di Catania, Italy

Humanity's interest in deep-space missions underscores the need for polymeric materials that can withstand harsh extraterrestrial environmental conditions. Polyetherimide (PEI) is attractive for aerospace structures because of its low density and mechanical robustness[1]. However, prolonged exposure to galactic cosmic rays, solar wind, and/or atomic oxygen causes erosion, mass loss, and deterioration of mechanical, thermal, and electrical properties[2]. Inorganic barriers (e.g. SiO_2, Al_2O_3, ZrO_2) offer hardness, chemical stability, and erosion resistance. Nevertheless, the lack of covalent anchoring of the coatings results in the loss of interfacial adhesion, delamination, and long-term stability.
Herein, we report a covalent silica-based self-passivating PEI system obtained through a multi-step functionalization[3]: partial hydrolysis of surface imide groups to obtain a polyamic acid (PAA) layer; chemical reduction of PAA's carboxyl to hydroxybenzyl moieties; grafting of tetraethyl orthosilicate to produce a silica-rich passivating layer. Each stage was monitored by ATR-FT-IR, UV-Vis DRS, contact-angle, and FE-SEM/EDX analyses.
The shielding efficacy was evaluated by exposing pristine and silica-modified PEI to simulated solar wind (protons at 200 KeV). Pristine PEI exhibited significant spectral and morphological changes due to on-surface erosion, whereas silica-modified PEI's surfaces retained silica signatures and microstructural integrity, even after ion bombardment at high fluence, indicating the effect of a strong self-passivating barrier.
Finally, to assess the applicability of the material in real-scenarios, a computer simulation was performed to estimate the energy dose for the proposed material as a function of the radius for different space orbits and on the moon's surface. Overall, our approach provides a straightforward and scalable route to improve the durability of polymers in space environments.

This work was funded by University of Catania (PIACERI 2 - MATTINATA).

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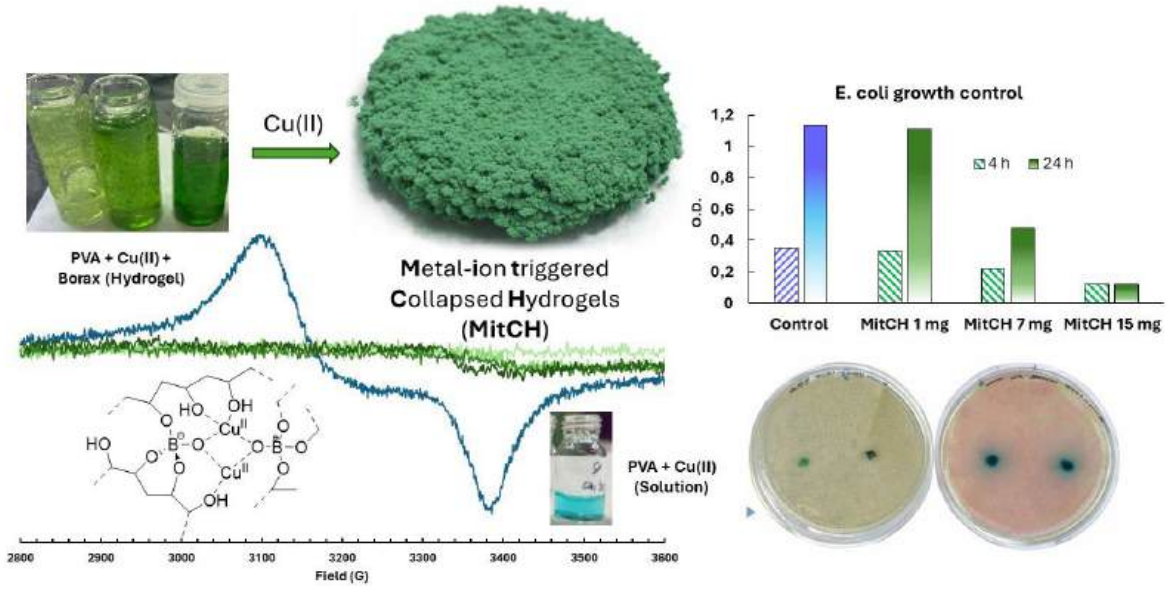
IM - D1 - P15
Metal ion-triggered collapsed hydrogels as new materials for bacterial population control

Danniel Gee[1], Roser Montagud-Martínez[2], Rosa Adam[1], Carlos J. Gómez-García[3], Guillermo Rodrigo[2], Rafael Ballesteros-Garrido[1]*
[1]Dept. of Organic Chemistry, Faculty of Chemistry, University of Valencia, Spain; [2]Instituto de Biología Integrativa de Sistemas (I2SysBio), CSIC-UV, Spain; [3]Dept. of Inorganic Chemistry, Faculty of Chemistry, University of Valencia, Spain

Hydrogels are versatile soft materials widely used in applications ranging from biomedicine to environmental technologies due to their high water content and tunable properties.[1] Herein, we report a metal ion-triggered collapse phenomenon in poly(vinyl alcohol)(PVA)–borax hydrogels induced by Cu(II) cations, leading to the formation of a new class of materials: Metal ion-triggered Collapsed Hydrogels (MitCH).[2] Upon increasing copper(II) sulphate concentration, conventional PVA–borax hydrogels undergo a sudden contraction expelling water and generating a rubbery, mechanically robust solid enriched in copper and boron species. Elemental and ICP analyses reveal copper loadings up to ~14 wt%, while sulphate is largely released during collapse, indicating extensive reorganization of the coordination environment. Structural characterization by PXRD, thermogravimetric analysis, diffuse reflectance spectroscopy, and EPR supports the formation of amorphous materials in which Cu(II) ions are coordinated by PVA hydroxyl groups and borate units, leading to antiferromagnetically coupled copper centers. The collapse process occurs under neutral pH conditions and is highly dependent on copper concentration, counterion identity, and PVA molecular weight and degree of hydrolysis. Importantly, MitCH materials are stable in water but dissolve in nutrient-rich biological media, enabling a smart, environment-responsive release of copper ions. This behavior was successfully exploited to control the growth of Escherichia coli, showing complete inhibition at sufficient material loadings. These results demonstrate that MitCH materials represent a promising platform for controlled antimicrobial applications, combining high metal loading, aqueous stability, and selective release triggered by biological environments.



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IM - D1 - P16
Form-factor free, liquid crystal-based gels for biosensors

Changyeon Lee[1], Jong Pil Park[2], Tae Jung Park[3], Chang-Hyung Choi[4]
[1]Dept. of Chemical Engineering, Chung-Ang University, Republic of Korea; *[2]Dept. of Food Science and Technology, Chung-Ang University, Republic of Korea*; *[3]Dept. of Chemistry, Chung-Ang University, Republic of Korea*; *[1]School of Chemical Engineering, Yeungnam University, Republic of Korea*

This study presents a strategy for the detection of biomolecules, including peptides and mRNA, using a liquid crystal gel (or nematogel) platform. The proposed system leverages the anisotropic optical properties, specifically the birefringence, of mesogens confined within a crosslinked polymer network to transduce molecular interaction between liquid crystals and targets into measurable optical signals. Unlike conventional liquid crystal-based biosensors that typically require glass-cell encapsulation or specific substrates, we fabricate free-standing and form-factor-free nematogels. We anticipate that these structural advantages enable the fabrication of the sensor in diverse geometries and its integration into various device configurations without the need for external supports.

This work was supported by a National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-02233102).

IM - D1 - P17

Rational design of lignin-derived bio-based plasticizers for sustainable polymer applications

Marina Pedrola[1], Ramon Meseguer[1], David Santiago[1]
[1]Eurecat, Centre Tecnològic de Catalunya, Unitat de Tecnologia Química, Spain

The global shift toward sustainable chemistry and a circular economy has intensified efforts to replace petroleum-based additives with biomass-derived alternatives.[1] In the polymer industry, this transition is essential for reducing environmental impact, and bio-based plasticizers play a key role in enhancing the performance and processability of PET and biodegradable polyesters such as PHA.

Plasticizers improve flexibility and melt flow by lowering the glass transition temperature (T*g*) and increasing chain mobility. Although phthalates have traditionally fulfilled this role, concerns about toxicity and environmental persistence have accelerated the search for safer options.[2] Bio-based plasticizers from renewable sources such as vegetable oils, fatty acids, and natural compounds offer non-toxic alternatives that tailor PET properties while reducing carbon footprint and meeting regulatory demands. However, advancement in this field is limited by the small range of available bio-based plasticizers.[3]

This study explores two novel families of lignin-derived additives, primarily vanillic and *p*-coumaric acids, with the aim of understanding how targeted structural modifications affect polymer behavior. To avoid covalent bonding with the polymer matrix and promote physical interactions, two strategies were applied: protecting phenolic groups through methylation and extending acidic functionalities with alkyl substituents of varying steric bulk. The versatility of these additives is further assessed by evaluating their performance in PHA and other bio-based polymers.

In summary, this work expands the design space of bio-based additives for PET, offering strategies to optimize performance, processability, and sustainability. The adaptable nature of their structures also reveals potential applicability beyond PET, advancing more circular and environmentally responsible polymer technologies.

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IM - D1 - P18
Sustainable anticorrosive pigments from mussels shell by-products

Nayara Balaba[1], Julia de O. Primo[1], Marjorie Olivier[2], Rafael Emil Klumpp[2], Carla Bittencourt[1]
[1]Plasma-Surface Interaction Chemistry (ChIPS) at the University of Mons, Belgium; [2]Materials Science Dept., Faculty of Engineering, University of Mons, Belgium

Mussel production, predominantly centered in Europe, yielded approximately 2 million tonnes in 2019, generating substantial quantities of by-products, with shells comprising 80–90% of the total mass[1]. The disposal and management of these shell residues are often inadequate, contributing to environmental challenges such as the emission of unpleasant odors, contamination from decomposing organic material, and visual pollution[2]. Nevertheless, the shells of bivalve mollusks are primarily composed of $CaCO_3$, making them a promising and sustainable alternative to commercial synthetic reagents in green chemical synthesis[2].
One important application of this waste is the green synthesis of metal phosphate pigments using CaO obtained from calcined mussel shells, phosphate salts, and chromophore ions. In this work, Mn or Ni ions were introduced as dopants to produce pigments with lilac and yellow hues, respectively (Figure 1). Phosphate-based pigments are widely recognized for their excellent anticorrosive properties, as they promote metal passivation by forming insoluble and adherent layers that hinder electrochemical reactions[3]. In particular, nickel- and manganese-based pigments are notable for their high chemical stability, low solubility, and effective anodic inhibition, resulting in durable corrosion protection[3,4].
We used different characterization techniques to confirm the properties of the synthesized pigments. XPS analysis of the Mn 2p and Ni 2p core levels (Figure 2a,b) revealed characteristic peaks corresponding to Mn^{3+}/Mn^{2+} and Ni^{3+}/Ni^{2+} oxidation states[5]. These oxidation states were confirmed by UV–Vis spectroscopy (Figure 2c,d), which also enabled band gap determination using the Kubelka–Munk method, classifying the pigments as semiconductors suitable for anticorrosive applications[6,7]. XRD analysis (Figure 2e,f) identified calcium hydroxyapatite (H-Ap) and β-tricalcium phosphate (β-TCP) as the main crystalline phases[8]. The absence of distinct Mn or Ni peaks indicates successful incorporation of the dopant ions into the H-Ap or β-TCP crystal structures[9], confirming effective waste-derived pigment synthesis with strong anticorrosive potential.

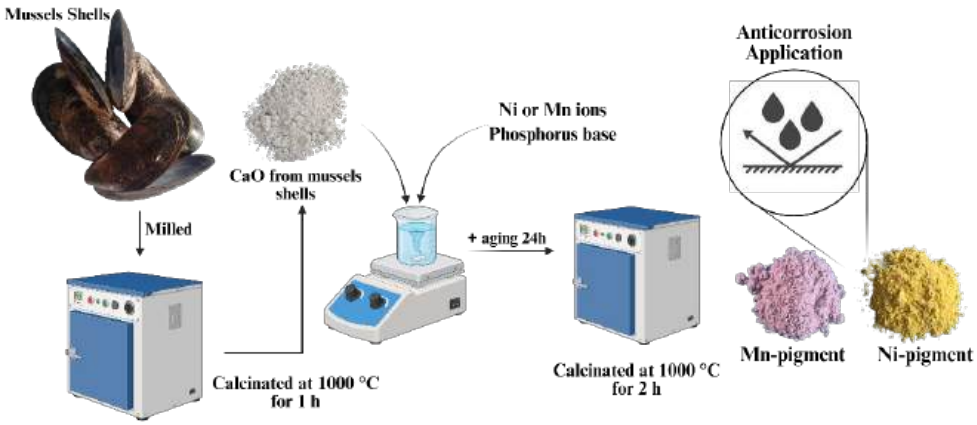

Fig. 1. Pigment synthesis schema: The synthesis was performed via a wet-chemical route. In the first stage, the mussel shells were milled and thermally treated to produce CaO. In the second stage, the reagents were dispersed in 50 mL of deionized water and homogenized under magnetic stirring for 2 hours. The resulting suspensions were calcined. The pigments were then dispersed in 0.5% and 2% epoxy resin (VossChemie) and applied to steel sheets to perform anti-corrosion tests.

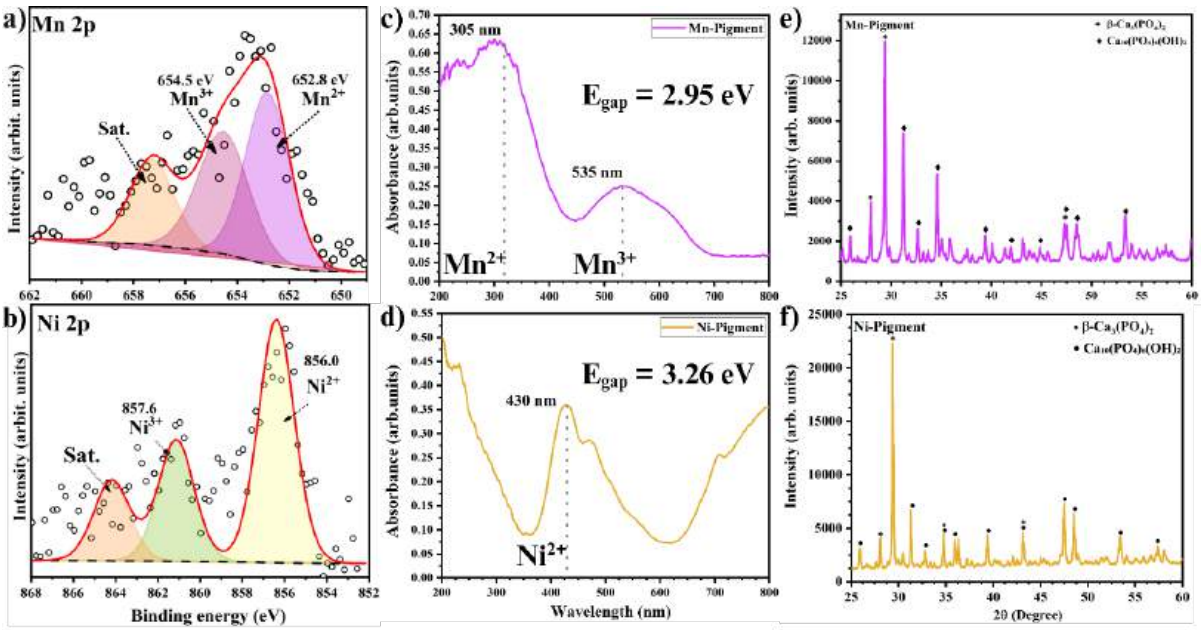

Fig. 2. Spectrum XPS for the (a) Mn-pigment and (b) Ni-pigment, where the binding energies were calibrated using the C1s peak (284.6 eV) as a reference. The detection of synthesized (c) Mn-pigment and (d) Ni-pigment was done in UV–UV-visible spectrophotometer by scanning the absorbance spectra in the range of 200–800 nm. The crystalline structure of the (e) Mn-pigment and (f) Ni-pigment was characterised by XRD, with a CuKα radiation source of λ = 1.5418 Å, potential of 40 kV, current of 30 mA, varying between 25- 60° (2θ), dwell time of 2 min^{-1} and step of 0.02 degrees.

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IM - D1 - P19

A curcumin-extract-containing copolymer as an optical sensor for volatile amines in smart food packaging applications

Angelo Nicosia[1], Lidia Mezzina[1], Placido Mineo[1,2]
[1]Dept. of Chemical Sciences, University of Catania, Italy; [2]Institute for Chemical and Physical Processes, National Research Council (IPCF-CNR), Messina, Italy

Volatile amines from natural and human-made sources are recognized as hazardous pollutants because of their irritative and carcinogenic effects. Food may also pose toxicological risks due to biogenic amines produced by microorganisms during spoilage and linked to inadequate storage[1]. Conventional analytical methods are accurate but unsuitable for rapid on-site detection. This pushes the development of optical sensors with real-time feedback that can be integrated into food packaging. In this context, Curcumin (extracted from *Curcuma longa*) is a natural dye with low toxicity and high sensitivity to pH, anions, and metal cations. However, its physical incorporation into polymer matrices often results in poor adhesion and dye leakage.

To overcome these limitations, we developed a copolymeric sensor in which Curcumin was covalently attached as a side-chain to a vinyl acetate-acrylic acid copolymer, followed by metalation with Zn(II) salt[2]. This synthetic approach ensures the stability of the sensing unit and its compatibility with food-related applications, leveraging the intrinsic adhesivity and low toxicity of the used copolymer. Comprehensive characterization was performed by NMR, UV-vis and fluorescence spectroscopies, GPC and thermal analyses.

Thin films of the Zn-Curcumin-containing copolymer were used as sensors for volatile organic compounds, showing excellent responses to nucleophilic species (ammonia, ethylenediamine, and pyridine) and negligible responses to weakly nucleophilic or nonpolar molecules (ethanol and toluene). The studied Curcumin-based copolymers emerged as cost-effective and scalable sensors for environmental monitoring and food packaging applications. This study represents the first application of Zn-Curcumin derivatives in colorimetric sensing, promoting Metals-Curcumin polymeric multisensor arrays for amine recognition.

This work was funded by the University of Catania (PIACERI 2 - MATTINATA, Linea di Intervento 2) and the European Union (NextGeneration EU, MUR-PNRR project SAMOTHRACE - ECS00000022).

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IM - D1 - P20
Phosphorylated lignin residues as a filler material for HDPE composites

Brian Claesen, Wouter Marchal
Hasselt University, Analytical & Circular Chemistry (ACC) group, Belgium; VITO, Belgium

In the ongoing shift towards a circular economy, considerable research efforts have recently been directed toward plant-based sourcing of essential chemicals, such as phenolics derived from technical lignin waste streams. However, during the work-up of this stream, a considerable amount of **insoluble solid (lignin) residues** is generated (up to 60 wt%) that adversely impacts the atom economy of this process. To address this challenge, we propose an innovative approach to convert these residues into valuable **flame-retardant fillers**. This mitigates the waste issue and aligns with the growing demand for bio-based halogen-free flame retardants, therefore, tackling two critical challenges simultaneously.
Importantly, we will also explore non-toxic and environmentally friendly phosphorylation reagents in this process that have not been reported yet in the literature. Two different types of lignin residues (**kraft and hydrolysis** origin) were investigated in terms of their characteristics and phosphorylation behavior. Until now, 4-5% of phosphorus has been introduced into the lignin residue matrix, and these phosphorylated lignin particles have been successfully incorporated into **HDPE**, aiming to produce a composite more prone to thermal degradation. Mechanical tests were performed to observe deterioration in toughness and maximum tensile strength compared with the 100% pure HDPE reference. However, elasticity was increased after introducing lignin particles into the HDPE matrix. The **UL94 horizontal burning test** was the final experiment conducted to assess the flame-retardant properties of the produced composites. The burning rates of the composites were compared with those of the HDPE reference.

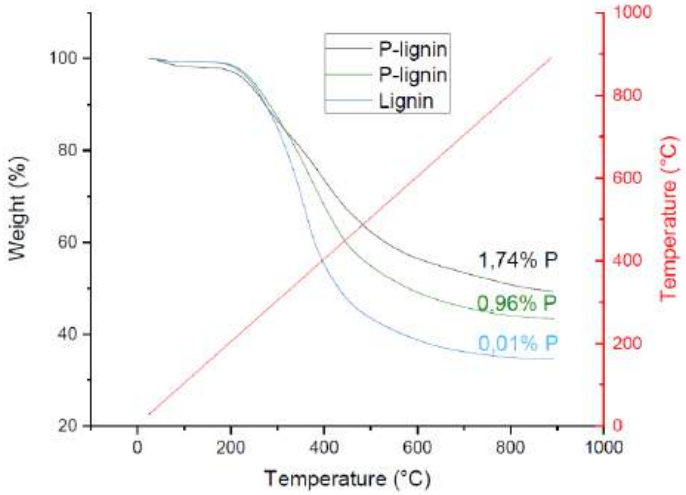

Fig. 4. Thermal gravimetric analysis (TGA) of a kraft lignin residue (Lignin) and two modifications enriched in phosphorus.

IM - D1 - P21

Engineering indenofluorenes with controlled diradical character and excited-state aromaticity toward singlet fission

Sergio Moles Quintero[1], Mercedes Alonso[1]
[1]Vrije Universiteit Brussel, Belgium

Singlet fission (SF) has emerged as a powerful approach to boost the performance of photovoltaic devices, as it enables the conversion of a single high energy photon into two triplet excitons, potentially surpassing the Shockley-Queisser efficiency limit. Despite its promise, efficient SF requires stringent energetic relationships between the relevant excited states. Organic molecules exhibiting inherent diradical character are particularly attractive in this context, since their electronic structure facilitates precise tuning of singlet–triplet energy gaps. Pentacene and tetracene derivatives, historically the most studied SF chromophores, offer the appropriate energy alignment but face notable challenges. Their limited chemical robustness, especially under ambient conditions, leads to rapid degradation and restricts their technological applicability. In contrast, many diradicaloid frameworks display exceptional environmental stability; some have even been implemented in OFETs or as photosensitizers. Moreover, in diradicaloids the energetic ordering of excited states arises from the balance between open-shell covalent and closed-shell ionic resonance forms, a feature that can be deliberately adjusted through molecular design. Among the available design strategies, aromaticity stands out as a key handle for fine-tuning excited-state energies.
In this study, we emphasize the potential of diradicaloids as SF-active materials and investigate their structure property relationships using computational methods. In particular, we focus on indenofluorene-based diradical systems, analyzing how aromaticity in both ground and excited states correlates with their diradical character and the associated excited-state energies. These insights establish a rational basis for designing next-generation indenofluorene-derived chromophores with optimized singlet-fission performance.

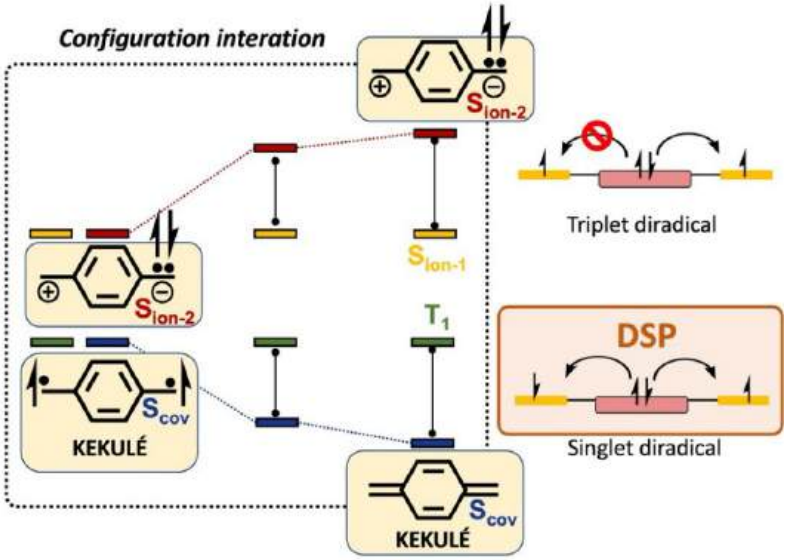

Fig. 1. Representation of how mixing between the covalent ground-state configuration and the ionic configurations modulates the energy distribution of the excited states, together with the double spin polarization (DSP) mechanism that stabilizes the singlet configuration relative to the triplet.

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IM - D1 - P22

Dual crosslinked printable chitosan/PEG/γ-cyclodextrin hydrogels with tunable rheological properties

Semih Macit[1], Emre Akar[2], Hakan Durmaz[2], Yasemin Yuksel Durmaz[1,3]

[1]School of Engineering and Natural Sciences, Istanbul Medipol University, Türkiye; [2]Dept. of Chemistry, Istanbul Technical University, Türkiye; [3]Research Institute of Health Science and Technologies (SABITA), Istanbul Medipol University, Türkiye

3D bioprinting is an innovative technology that enables the layered production of living tissues, organs, and biomimetic structures. This technology is inspired by traditional 3D printing technologies but unlike them, it uses a special ink that allows cell adhesion. It is critical that these bioinks possess suitable rheological and mechanical properties that ensure fluidity during printing and maintain structural integrity after printing. In this study, printable hydrogel systems containing chitosan (Ch), poly(ethylene glycol) derivatives, and γ-cyclodextrin (γCD) with different crosslinking mechanisms were developed. The hydrogel systems were prepared using covalent crosslinking approaches based on amino-yne "click" reactions with PEG-DA and divinyl sulfone (DVS) as crosslinker, and combinations of these two systems were also investigated.[1] In addition to primary covalent bonds, hydrogen bonds formed through the hydroxyl groups of γCD provided secondary physical interactions, contributing to the structural integrity of the system. Thanks to this double crosslinking approach, flow was achieved by breaking physical bonds during printing, while covalent bonds and recovered hydrogen bonds maintained the stability of the structure after printing. Rheological analyses showed that the developed hydrogel systems exhibited a self-supporting structure with storage modulus in the range of 10^3–10^4 Pa and tanδ<1 values as shown in **Table 1**. Furthermore, it was determined that the systems exhibited shear thinning and thixotropic behavior. SEM analyses revealed that the hydrogels have a porous and interconnected internal structure. The findings indicate that the developed hydrogel systems are promising candidates for tissue engineering and biomedical applications.

Table 1. Rheological results of hydrogels.

Gel	η (Pa.s)	Max G' (Pa)	tanδ	Gelation T (℃)	90% Recovery (s)
CPGT1	516.8	3165.6	0.2	27.4	10
CPGT2	792.8	4812.9	0.3	28.5	25
CPGT3	1600	9790.4	0.2	20.0	5
CPdGD3	731.7	4533.9	0.2	32.7	9
CPdGD4	1349.2	8208.1	0.3	27.4	38
CPdGD5	250.4	1553.3	0.2	27.4	10

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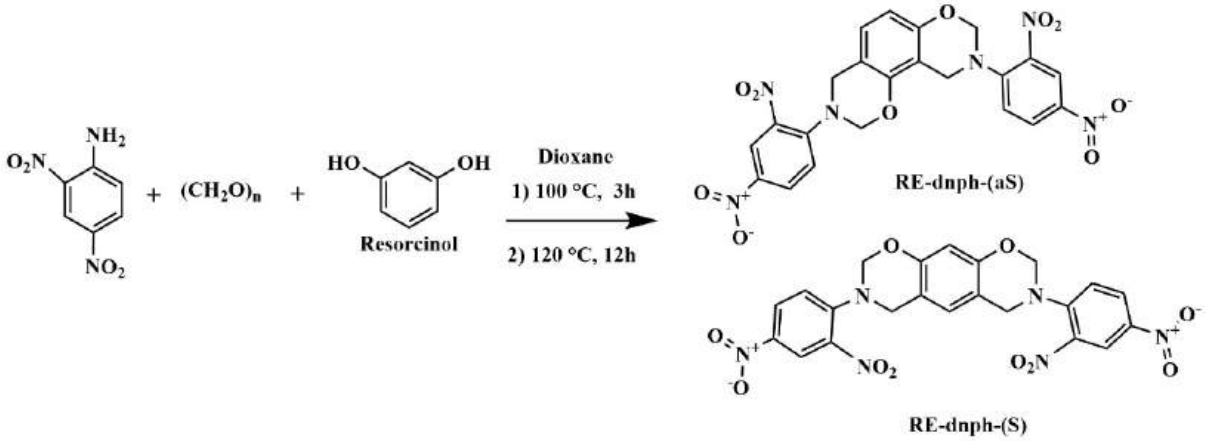
IM - D1 - P23
Lightweight energetic polymers for next-generation ammunition

Slimane Abdous[1], Mehdi Derradji[2], Oussama Mehalli[3]
[1]UER Procédés Energétiques, Ecole Militaire Polytechnique, Bordj El-Bahri, Algiers Algeria

Modern ammunition typically includes around 30% explosive material, while the majority of its weight comes from structural metals like steel and aluminum that don't contribute to the energy output [1-3]. Reactive structural materials (RSMs) aim to enhance performance by combining mechanical strength with energetic properties [4]. High-strength polymers with glass transition temperatures above operational limits are emerging as promising replacements for conventional metal components [5]. In this study, an energetic polymer based on resorcinol and 2,4-paranitroaniline benzoxazine (RE-dnph) was synthesized and evaluated **Scheme 1**. The material demonstrated robust performance, including deflagration temperatures between 260–265 °C and an energy release of 23.33 $kJ \cdot g^{-1}$ **Table 1**. Thermal analysis via DSC-TGA confirmed its potential use in RSMs, providing both structural durability and significant energy release.



Scheme 1. Synthesized symmetric and asymmetric RE-dnph monomers.

Table 1. Physical and energetic data of the RE-dnph benzoxazine polymer.

Sample	RE-dnph
Formula (repeating unit)	$C_{22}H_{18}N_8O_{10}$
Molecular weight (g·mol-1)	554
Appearance	Reddish powder
Heat of combustion -ΔUcomb (kJ·g-1)	23.33
Enthalpy of combustion -ΔHcomb (kJ·mol-1)	1775.82
Heat of formation -ΔfH (kJ·mol-1)	9466.18
Oxygen balance OB (%)	-124.18

Deflagration temperature Tdef (°C)	261
Density ρ (g·cm-3)	1.59

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IM - D1 - P24
Ionic liquids: A new way in the preparation of sustainable PBSA nanobiocomposites

Housséem Chabane[1], Zineddine Bensalem[1], Halima Saadiya Ababsa[1], Ahmed Mekki[1], Sébastien Livi[2]
[1]Laboratoire de Chimie Macromoléculaire, Ecole Militaire Polytechnique (EMP) CHAHID ABDERRAHMANE TALEB, Algeria; [2]Université de Lyon, CNRS, Université Claude Bernard Lyon 1, INSA Lyon, Université Jean Monnet, UMR 5223, Ingénierie des Matériaux Polymères, France

The 21st century is often referred to as the “Age of Plastics” where the mass consumption of disposables leads to excessive pollution and contributes to the climate crisis. Indeed, single-use plastics are frequently used for packaging applications. Thus, in line with political and ethical demands of our times, scholars and industries are pushed to search for sustainable materials. In this work, a new generation of nanocomposites were prepared by melt mixing using poly(butylene succinate-co-adipate) (PBSA) as matrix reinforced with 5 wt. % of POSS®^{Ph} nanoclusters, i.e. unmodified trisilanol phenyl POSS® (POSS^{Ph}-triol) and two prepared ionic liquid-modified POSS®^{Ph} (IL-g-POSS^{Ph}) having chloride (Cl^-) or bis-trifluoromethanesulfonimidate (NTf_2^-) counter anions, in order to develop more sustainable and efficient active packaging food systems. The incorporation of IL-g-POSS^{Ph} into PBSA matrix led to the formation of well-dispersed POSS nanoclusters (10 to 100 nm) resulting in a significant increase of the mechanical performances, i.e., Young’s modulus (982 vs 260 MPa) and strain at break (297 vs 226 %). In addition, the corresponding PBSA nanocomposites displayed outstanding water (87 %) and oxygen (90 %) barrier properties combining with higher bactericidal and fungicidal activities. Finally, biodegradation tests under soil burial conditions showed a better ability of the PBSA nanocomposites to biodegrade after 12 weeks (84 against 58 % for pure PBSA).

Keywords: Poly(butylene succinate-co-adipate), Ionic Liquids, Polyhedral Oligomeric Silsesquioxane (POSS), Mechanical performances, Biodegradation, Antibacterial activity.

IM - D1 - P25

Interfacial effects of monomeric and dimeric surfactants in waste-oil microencapsulation for advanced self-healing materials

Mohammed Siddiq Abdul Rahim[1], Muhammad Faizan Khan[2], Mohammed Ali Alosta[3]

[1]Interdisciplinary Research Center for Construction and Building Materials, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia; [2]Dept. of Bioengineering, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia; [3]Dept. of Civil and Environmental Engineering, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia

Interfacial phenomena play a decisive role in the microencapsulation of liquid cores for advanced self-healing material systems. In this work, the interfacial effects of monomeric and dimeric surfactants on the microencapsulation of waste-derived oils were systematically investigated to develop sustainable healing agents for advanced self-healing materials. Waste cooking oil (WCO) and waste engine oil (WEO) were utilised as core materials and encapsulated through acid-catalysed in situ polymerisation. Three surfactant systems with distinct molecular architectures were examined: monomeric anionic sodium dodecyl sulfate (SDS) and two dimeric (gemini) cationic surfactants, namely COCO gemini (16-6-16 adipate) and GS12. Emphasis was placed on correlating surfactant charge, molecular structure, and adsorption behavior with emulsion stability, interfacial robustness, and polymer shell formation. The results demonstrate that monomeric anionic SDS provides strong electrostatic stabilization under acidic conditions, leading to stable oil-in-water emulsions and uniform microcapsules for both waste oil types. In contrast, dimeric cationic surfactants exhibited pronounced interfacial destabilization during polymerization, particularly in low-pH and high-ionic-strength environments, resulting in oil coalescence and incomplete shell formation. These effects are attributed to unfavorable interfacial interactions and charge repulsion during polymer growth. The incorporation of a nonionic co-surfactant introduced steric stabilization at the oil-water interface, significantly improving emulsion stability and enabling successful encapsulation in dimeric surfactant systems. Overall, this study elucidates how interfacial effects governed by surfactant molecular architecture control waste oil microencapsulation outcomes. The findings provide molecular-level insights for the rational design of microcapsules and demonstrate a viable pathway for transforming waste oils into functional components for advanced self-healing materials, contributing to sustainable and durable material technologies.

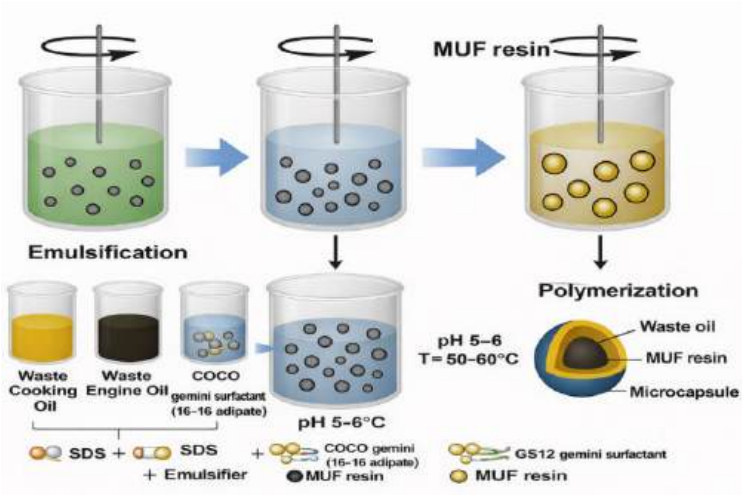

Fig. 1. Schematic of the synthesis process of microcapsules containing WCO and WEO by in situ polymerization.

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IM - D2 - P01
Can POSS be used as radiative cooling materials?

Patrycja Wytrych[1], Urszula Malecka[1], Alexander Korneluk[1], Tomasz Stefaniuk[1]
[1]*University of Warsaw, Poland*

Radiative cooling is a passive and energy-efficient method of dissipating heat, relying on the emission of thermal infrared radiation from a material's surface into the cold sink of outer space. This effect takes advantage of the atmospheric transparency window between 8 and 13 μm, where infrared absorption by atmospheric components is minimal, allowing heat to be effectively radiated away from Earth. By utilizing this natural pathway, radiative cooling enables temperature reduction without external power input, offering a sustainable solution for thermal regulation **across** a wide range of applications.
The performance of radiative cooling systems depends strongly on the optical and physicochemical characteristics of the materials involved. In this context, **polyhedral oligomeric silsesquioxanes (POSS)** are examined as promising candidates. POSS molecules consist of a distinctive silicon–oxygen cage that can be functionalized with numerous substituents, **ranging from** simple hydrogen atoms **to** complex organic groups. This hybrid inorganic–organic architecture imparts the thermal and chemical robustness typical of silica, while the surrounding organic moieties provide mechanical flexibility and enable extensive chemical tunability.
Our study demonstrates that POSS-based materials possess a compelling combination of infrared emissive properties, durability, and structural adaptability, making them well suited for radiative cooling technologies. Ellipsometric analysis shows that POSS exhibits **high** thermal emissivity in the infrared region coupled with low absorption of solar irradiation, both essential for effective passive cooling. The optical and physicochemical behavior of POSS varies significantly with the type and number of functional groups, including reactive moieties such as vinyl or amino groups, as well as inert substituents like isobutyl or methyl groups. Moreover, their mechanical resilience, weather resistance, and ease of fabrication further support the use of POSS as advanced materials for next-generation cooling applications.

IM - D2 - P02
Structural diversity in γ-CD-MOFs: Two new polymorphs

Stijn Germonpré[1], Kristof Van Hecke[1]
[1]XStruct, Department of Chemistry, Ghent University, Belgium

Two new polymorphs of the potassium γ-cyclodextrin metal–organic framework (K-γ-CD-MOF) have been synthesized and structurally characterized. While the well-known K-γ-CD-MOF typically crystallizes in a cubic system[1], these novel forms adopt orthorhombic ($P2_12_12_1$, γ-CD-MOF-3) and monoclinic (C2, γ-CD-MOF-2) symmetries. Both polymorphs retain the characteristic γ-CD toroidal units[1], but differ significantly in packing, channel orientation, and pore connectivity.
Crystallization was achieved via controlled vapor diffusion, with slight variations in solvent and temperature yielding distinct frameworks. Single-crystal X-ray diffraction (SCXRD) confirmed their unique crystal packings and topologies.

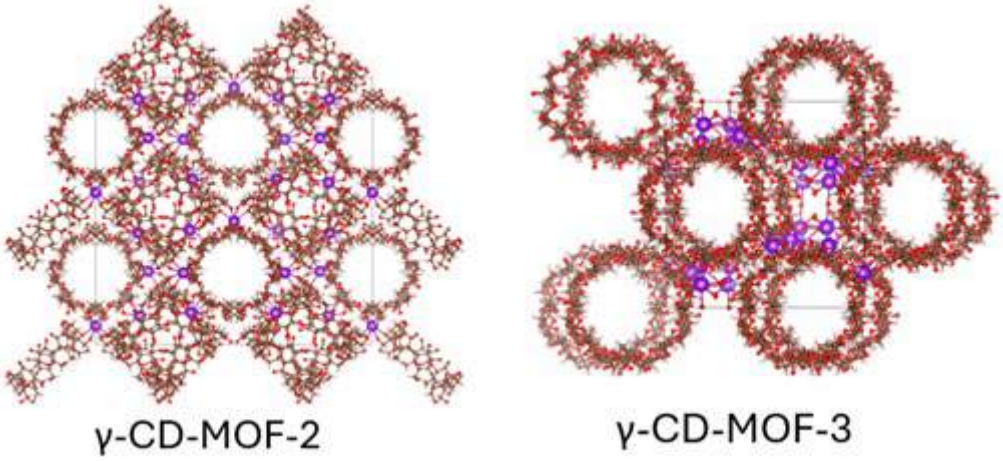

Figure 1: SCXRD crystallographic packing units of different γ-CD-MOF polymorphs.

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IM - D2 - P03

Surface characterization and daylight-activated antibacterial performance of ZN(II) phthalocyanine-coated titanium

Ece Tuğba SAKA[1], Salih DURDU[2], Kadriye ÖZCAN[3], Yasemin ÇAĞLAR[3]
[1]Karadeniz Technical University, Dept. of Chemistry, Turkey; [2]Giresun University, Dept. of Industrial Engineering, Turkey; [3]Giresun University, Dept. of Genetics and Bioengineering, Turkey

Titanium and its alloys are widely used in biomedical and engineering applications due to their excellent mechanical properties, corrosion resistance, and biocompatibility; however, their susceptibility to bacterial colonization and biofilm formation remains a significant challenge. Surface modification strategies have therefore gained considerable attention as an effective approach to impart antibacterial functionality without compromising the bulk properties of titanium. Among these strategies, phthalocyanine-based coatings are particularly attractive due to their strong absorption in the visible region and their ability to generate reactive oxygen species under light irradiation [1-2].

In this study, Zn(II) phthalocyanine [3] was coated onto titanium surfaces using the drop-casting method with a dimethylformamide (DMF) solution. Following coating, XRD, SEM, EDX, FTIR and contact angle measurement tests were performed. The phthalocyanine-coated surfaces exhibited greater hydrophobicity than the uncoated surfaces. Activity tests against *E. coli* and *S. aureus* bacteria were then performed on the coated surfaces under both dark and daylight conditions. The phthalocyanine-coated titanium surfaces showed over 90% inhibition of these organisms under daylight conditions.

This work was supported by Karadeniz Technical University, Trabzon, Turkey, under Scientific Research Projects Coordination Unit (Project Number: FEN-BAP-A-250925-65).

Keywords: Zn(II) phthalocyanine, coating, titanium, antibacterial performance

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IM - D2 - P04

Nanocellulose extraction and valorization from spent coffee grounds for primary and secondary packaging

Carmen Corea[1], Laura Riva[1], Laura Gallo[2], Carlo Punta[1]
[1]Politecnico di Milano, Italy; [2]Coffeefrom Srl, Italy

Cellulose is a linear homopolymer composed by D-glucopyranose units linked via β-1,4 glycosidic bonds. The high number of hydroxy groups confers to cellulose a strong hydrogen bonding ability, facilitating the formation of microfibrillar crystalline regions. These crystalline domains impart high strength, stiffness and durability. Furthermore, the presence of primary hydroxy groups on C6 position allows cellulose to act as a versatile substrate, enabling the introduction of lipophilic groups to modify its hydrophilic nature[1]. In addition, the hierarchical structure of cellulose enables the extraction of nanoscale materials, among these, tempo-oxidized nanofibers (TOCNF) with a diameter in the range 3-100 nm, that can be extracted from both virgin and waste-derived materials[2].
In a recently licensed patent nanocellulose is extracted from spent coffee grounds (SCG) addressing the advantages in using an abundant waste as a feedstock[3]. In fact, approximately 20 million tons of SCG are generated yearly worldwide, containing around 30%w/w of cellulose[4]. The process described in the patent has been further optimized by adding an oil extraction step in which another product can be recovered.
This study focuses on the application of the different solid fractions obtained throughout the process in packaging industry, for primary and secondary packaging.
Defatted SCG was used for compounding with different polymers, in presence and in absence of TOCNF. The exhibited results in terms of permeability, thermal and mechanical properties were promising with respect to the current widespread technology, which involves using untreated SCG for compounding in PP and PLA.
Moreover, some preliminary results about active packaging formulation were collected, also making an attempt in extracting and reusing the polyphenolic fraction of SCG.

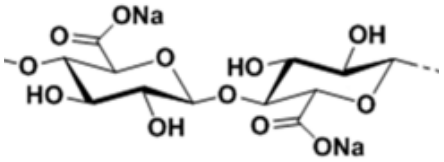

Fig.1 TOCNF repeating unit.

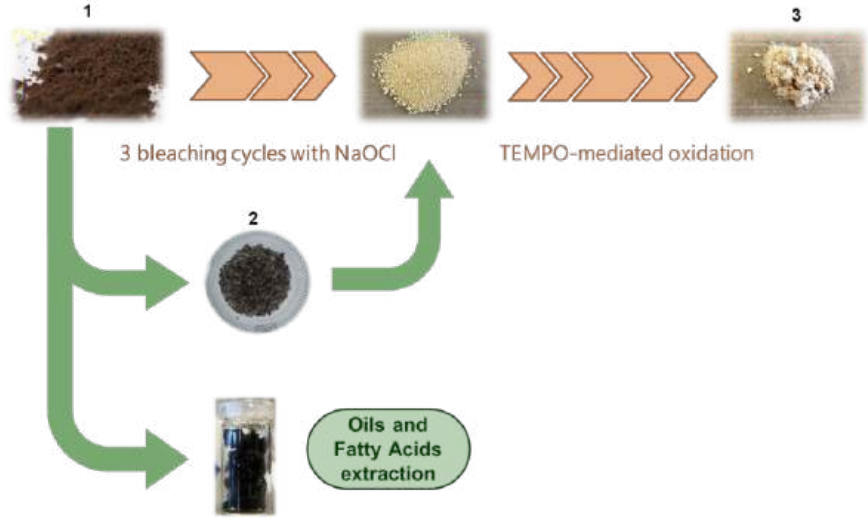

Fig.2 Valorization process scheme.

The author wishes to thank Coffeefrom Srl and the European Union NextGeneration EU (National Recovery and Resilience Plan_NRRP): Mission 4, Component 2, Investment 3.3_DM n. 630/2024 for the funding and facilities.

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IM - D2 - P05

Understanding the molecular interaction mechanisms of wine-waste pigments and biomordants to produce dyed sustainable wool textiles

Mário Pinho[1], Nuno Mateus[1,2], Victor Freitas[1,2], Natércia Teixeira[2]
[1]Faculty of Sciences, University of Porto, Portugal; [2]LAQV-REQUIMTE, Portugal

The wine industry generates massive quantities of solid waste annually[1], posing environmental challenges while offering significant opportunities for biotechnological valorization. This work focuses on repurposing red grape pomace (Vitis vinifera L.) as a source of anthocyanins—natural phenolic pigments with high coloring potential. Aligned with the European Green Deal, this research contributes to the development of sustainable materials through innovative, biodegradable, and ecological solutions.

Since the textile industry is one of the most polluting in the world[1-2], with synthetic dyeing being a major contributor, there is an urgent need for sustainable alternatives. Given the high dyeing potential of compounds in wine by-products, this work is the first systematic study on the use of these residues as natural dyes and biomordants. As wool is the best fiber for natural pigments[3], it serves as the primary focus of this investigation.

The research started by extracting these compounds from various grape varieties, followed by characterization using HPLC-DAD, HPLC-ESI/Orbitrap-MS, and NMR. This allowed for the identification of known monomeric anthocyanins and new polymeric colored species. Furthermore, the interaction between these extracts and wool fibers was investigated using Isothermal Titration Calorimetry (ITC) to assess chemical affinities and the underlying mechanisms.

To optimize color fixation and ensure a fully circular process, natural mordants derived from wine industry residues were explored, namely white wine extracts and tartaric acid (tartar) recovered from barrels and vats. Preliminary results indicate that tartaric acid effectively modulates the dyeing pH and enhances the chemical bonding between anthocyanins and wool keratin, improving colorfastness.

This project demonstrates the feasibility of transforming winery residues into high-value resources, providing a bio-based alternative to synthetic dyes while establishing new methods to optimize natural dyeing within a circular economy framework.

Acknowledgements: PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos. NT thanks FCT for the Scientific Employment Stimulus - Individual Call 2023.06024.CEECIND/CP2842/CT0010.
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IM - D2 - P06

Dependence of the optical properties of solid-state fluorescent carbon dots on temperature

Spyridon N. Katsantonis[1,2], Spiros Gardelis[3], Maryam Adnan[4], Yaaqoub Malallah[4], Marko Bošković[5], Danijela Randjelovic[5], Konstantinos V. Kordatos[1], Christos Tsamis[2]

[1]Dept. of Chemical Sciences, School of Chemical Engineering, National Technical University of Athens (NTUA), Greece; [2]Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research (NCSR) "Demokritos", Greece; [3]Condensed Matter Physics Section, Physics Dept., National and Kapodistrian University of Athens (NKUA), Greece, [4]Energy and Building Research Center, Kuwait Institute for Scientific Research, Kuwait, [5]Institute of Chemistry, Technology and Metallurgy (ICTM), National Institute of the Republic of Serbia, University of Belgrade, Serbia

Abstract

Carbon dots (CDs) are a class of carbon-based nanomaterials with excellent optical properties, biocompatibility and facile synthesis route. Depending on the selected precursor materials during the synthesis process, heteroatoms, like N, P, S and B, can be doped into the structure of CDs, thus leading to modification of their properties, including their photoluminescence [1]. Additional parameters that influence the photoluminescence of CDs are the excitation wavelength, pH value, solvent use and temperature [2–4]. Although the fact that the photoluminescence of CDs in solution-form has been extensively studied, in solid-state it still remains challenging due to fluorescence quenching caused by aggregation [5]. The aim of this work is to study the optical properties dependence of solid-state fluorescent CDs in correlation to temperature. Different types of CDs (N-doped, P-doped, N,P-co-doped) were synthesized by solvothermal treatment and deposited on SiO_2 substrates by spin coating, thus forming a thin film. The effect of temperature on the fluorescence of the different types of CDs in solid-state was studied by measuring the photoluminescence intensity in the temperature range of 300-360 K at 10 K intervals. Moreover, the structure and properties of the synthesized CDs were further analyzed by Fourier-Transform Infrared spectroscopy (FT-IR), Ultraviolet-Visible spectrometry (UV-Vis) and High-Resolution Transmission Electron Microscopy (HRTEM) and X-ray Fluorescence (XRF).

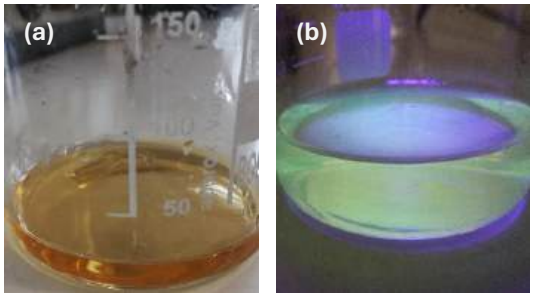

Figure 2 Solution of P-doped CDs under (a) natural light and (b) UV light.

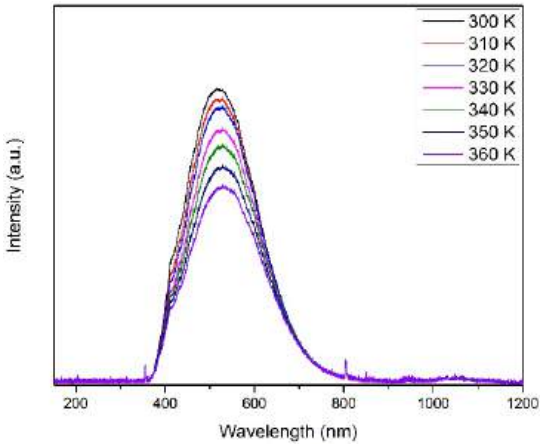

Figure 2 Photoluminescence spectra of P-doped CDs at different temperatures (300-360 K).

Acknowledgements

This research was sponsored by the NATO Science for Peace and Security Programme under grant id. [G7264].

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IM - D2 - P07

Heparin-binding domains in elastin-like proteins: A way towards improved tissue integration?

Niels Geysmans[1], Lotte Vastmans[2], Virginie Bito[2], Geert-Jan Graulus[1]
[1]Biomolecule Design Group, Institute of Materials Research, Hasselt University, Belgium; [2]CARDIOLab, Biomedical Research Institute, Hasselt University, Belgium

A heart attack leads to irreversible damage to the heart muscle. Current treatment methods primarily focus on preventing secondary infarcts but do not address the sustained tissue damage. Consequently, a myocardial infarction often initiates an unfortunate chain of events leading to the development of cardiac arrhythmias and ultimately heart failure. New stem cell therapies are under development, but their effectiveness is limited by the poor retention of these cells at the infarct site. As a result, the majority of injected cells do not have ample time to differentiate into functional cardiomyocytes. Injectable hydrogels provide an effective approach to enhancing stem cell retention. Elastin-like proteins (ELPs) have a long history in this field due to their intrinsic lower critical solution temperature (LCST).[1] In this contribution, we describe the design and biotechnological production of recombinant ELPs incorporating heparin-binding domains (HBDs). HBDs are a class of positively charged peptide domains that have been previously studied as an affinity tag in protein purification. The expected interaction of these peptide domains with negatively charged components of the extracellular matrix (ECM), such as hyaluronic acid and sulphated glycosaminoglycans (GAGs), is hypothesised to contribute to improved tissue integration of the stem cell carrier. In this presentation, we describe the optimised expression parameters, the validation of the proteins' LCST behaviour and their preliminary biocompatibility assessment. Finally, the ELPs' interaction with negatively charged ECM components was studied via lap shear tests.

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IM - D2 - P08

Bridging photoswitch and fluorescence features in artificial amphiphiles for membrane dynamics in liposomal vesicles

†Simone Cataldini[1], †Paola Albanese[1,4], Simona Amoroso[1], Lucia Sessa[2], Stefano Piotto[2], Miriam Di Martino[2], Simona Concilio[2], Ilektra Mavromatidou[1], Mohinder M. Naiya[5,6], Jlenia Brunetti[3], Emiliano Altamura[7], Agnese Magnani[1], Jack Li-Yang Chen[1,5,6], Federico Rossi[4]

[1]Dept. of Biotechnologies, Chemistry and Pharmacy, University of Siena, Italy; [2]Dept. of Pharmacy, University of Salerno, Italy; [3]MedBiotech Hub and Competence Centre, Dept. of Medical Biotechnologies, University of Siena, Italy; [4]Dept. of Physical Science, Earth and Environment University of Siena, Italy; [5]School of Science, Auckland University of Technology, New Zealand; [6]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand; [7]Department of Chemistry, University of Bari "Aldo Moro", Italy.

Natural cells stand as main compelling example of systems exhibiting remarkable stimuli-responsive capabilities. Scientific literature provides uncountable examples of supramolecular entities able to respond to controllable triggers, out of which light occupies a privileged position.[1] The integration of molecular switches and motors in membranes alters the membrane biophysics, leading to controllable supramolecular effects and life-like phenomena.[2] Throughout this work, a library of azobenzene-decorated amphiphiles was synthesized, following their embedment in the bilayer of liposomal carriers. By leveraging the (*E*)-*to*-(*Z*) photoisomerisation of engineered giant unilamellar vesicles (GUVs), microscopy experiments revealed distinctive supramolecular phenomena, spanning from reversible transitions in shape and size, and enhanced permeability to small polar molecules.[3] Further on, our endeavours focussed on novel analogues featuring both photoswitch and fluorescence. Several fluorescent scaffolds were screened, ultimately leading to a library of Nile Red-based (Ex_{max} = 515 to 559; Em_{max} = 585 to 635 nm) amphiphiles. The utilized fluorescent tag allowed to follow the molecule intercalation within the bilayer of both GUVs and LUVs, delving into analysis of membrane domains, supramolecular shape-transitions, and cargo-release experiments.

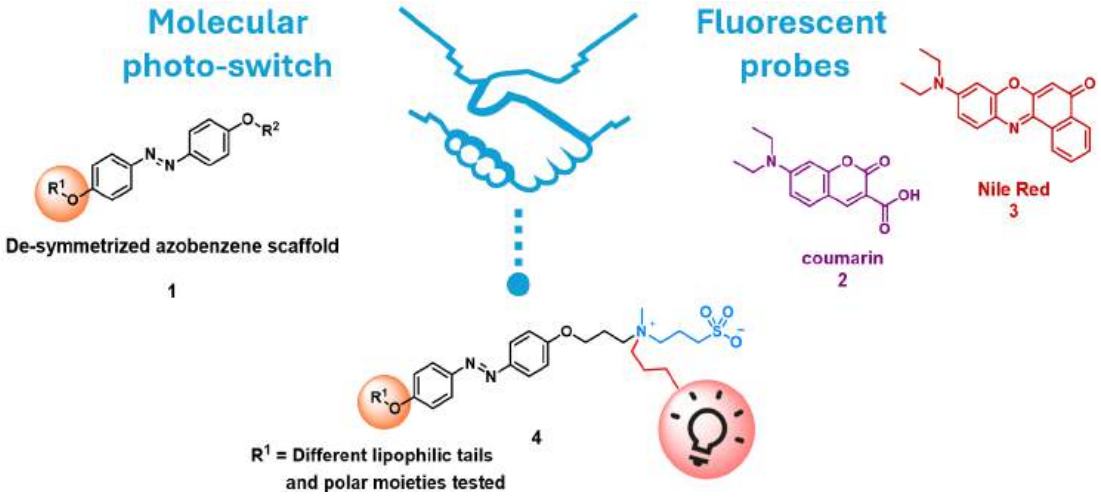

Figure. Schematic depiction of the combination of the azobenzene scaffold and fluorophores within the current work

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IM - D2 - P09

Zinc-based BIAN complexes and hydrogen-bonded organic frameworks: Sustainable photocatalysts for water-splitting hydrogen production

Jorge Maçãs[1], Vitor Rosa, Inês Matos[1], Sandra Gago[1], Clara S. B. Gomes[1]
[1]LAQV-REQUIMTE, NOVA School of Science and Technology, NOVA University of Lisbon, Portugal

While the global demand for hydrogen is surging, nearly 95% of its production still relies on fossil fuels, a process that remains carbon-intensive and fundamentally unsustainable. Solar-driven photocatalytic water-splitting offers a compelling, carbon-free alternative, yet the field is currently bottlenecked by the search for photocatalysts that are simultaneously efficient, durable, and cost-effective.[1]

Herein, we developed zinc-based supramolecular systems derived from [Zn(Aryl-BIAN)$_2$] complexes (Aryl-BIAN = bis(*p*-hydroxyphenylimino)acenaphthene; X = Cl, I) as visible-light-active photocatalysts for hydrogen production (Figure 1). These complexes and their corresponding hydrogen-bonded organic frameworks (HOFs) were synthesised using conventional solution-based routes and mechanochemical methodologies. This highlights mechanochemistry as a sustainable, solvent-minimised strategy for preparing functional, innovative photocatalytic materials.

By utilizing mechanical force to drive chemical reactions, we were able to enhance sustainability by significantly reducing solvent waste and improving energy efficiency, and scale efficiently by demonstrating a streamlined methodology for producing functional, innovative materials.

To address the challenges of catalyst recovery and long-term stability, we immobilized these complexes and HOFs onto solid supports, specifically mesoporous silica (MCM-41) and activated carbon (NORIT GAC 1240W). These hybrid materials transition the catalysts from homogeneous to heterogeneous systems, facilitating easier recycling and improved structural integrity during operation.

The structural and optical properties of the resulting materials were analyzed using various techniques, including X-ray diffraction (SCXRD and PXRD), FTIR, NMR, and diffuse reflectance spectroscopy (DRS). Finally, we evaluated the photocatalytic efficacy of these systems by measuring hydrogen evolution rates under visible-light irradiation, utilizing various sacrificial agents to optimize the water-splitting process.[2]

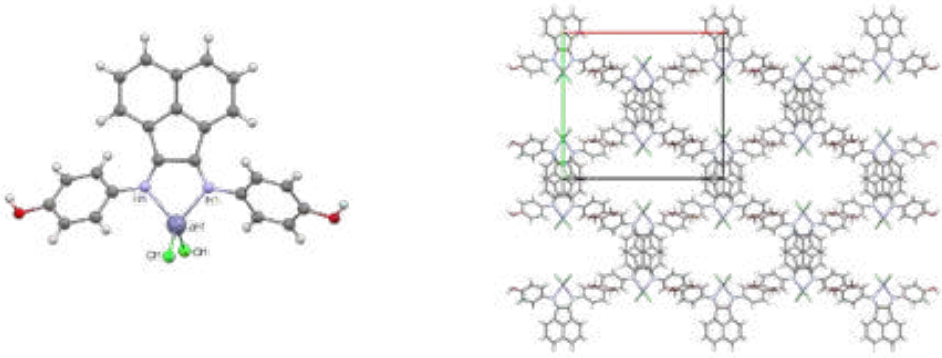

Figure 1. [Zn(Aryl-BIAN)Cl$_2$] (left) and its supramolecular arrangement viewed along the *c* axis (right).

This work was supported by FCT/MCTES through projects UID/50006/2023 and LA/P/0008/2020 (https://doi.org/10.54499/LA/P/0008/2020) and contract 2023.11076.TENURE.117, and by EU project IMPACTIVE (no. 101057286).

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IM - D2 – P10

Heterogenization of metal catalyst on carrageenan polysaccharides for sustainable synthesis

Adi Wolfson[1], Oshrat Levy-Ontman[1]

[1]Chemical Engineering Department, Sami Shamoon Collage of Engineering, Be'er Sheva, Israel

Renewable and biodegradable organic biopolymers, particularly polysaccharides, have found widespread applications across various industries, including pharmaceuticals, biomedical materials, cosmetics, and food. Owing to their unique structures and diverse functional groups, polysaccharides have also attracted increasing attention over the past decade as supports for metal catalysts. Yet, the heterogenization of metal complexes on polysaccharides to combine the advantages of homogeneous catalysis (high activity and selectivity) with those of heterogeneous catalysis (easy separation and recycling), depends on the structure and the properties of both the polysaccharide and the metal complex.

Polysaccharides can form two types of solid support: hydrogels, which are cross-linked polymeric networks produced by various agents such as metals or bases, and xerogels, which are dry, solid supports obtained by removing the liquid phase of a gel through evaporation using different techniques. Both forms can be employed as supports for metal catalysts, with their structural characteristics and physicochemical properties playing a key role in determining catalytic performance.

Herein, we report a simple and straightforward method for the preparation of heterogeneous metal catalysts based on carrageenans, a specific class of polysaccharides produced by red algae and characterized by ester sulfate groups along their backbone. The resulting heterogeneous catalysts incorporating palladium, rhodium, or ruthenium were successfully applied and recycled in a range of organic transformations, including olefin metathesis, Suzuki cross-coupling, transfer hydrogenation of olefins, aerobic oxidation of benzylic alcohols, and the Heck reaction. The new catalysts were also thoroughly characterized to elucidate the interactions between the metal species and the polysaccharide matrix and to gain insight into the structure of the resulting composites. Characterization was carried out using FTIR, SEM-EDS, XPS, SEM, TEM, TGA, and zeta potential analyses.

IM - D2 – P11

From waste to value-added polymers: Chemical transformation of PET into eco-friendly copolyesteramides

Makram Elabed[1,2], Slim Salhi[1], Pieter Billen[2], Philippe Nimmegeers[3,4,5], Houcine Ammar[1]
[1]Laboratory of Applied Chemistry (HCGP), Faculty of sciences, University of Sfax, Tunisia; [2]iPRACS research group, Faculty of Applied Engineering, University of Antwerp, Belgium; [3]Dept. of Engineering Management, Faculty of Business and Economics, University of Antwerp, Belgium; [4]Flanders Make@UAntwerp, Belgium; [5]NANOlight Centre of Excellence, University of Antwerp, Belgium.

The growing accumulation of polyethylene terephthalate (PET) waste is a major environmental challenge, stimulating research into advanced chemical upcycling strategies that go beyond simple recycling to generate high value-added materials. [1]

In this context, copolyesteramides (PEAs) appear to be a promising but still largely unexplored class of materials, synergistically combining the mechanical and thermal properties of polyesters with the chemical resistance and intermolecular interactions characteristic of polyamides. [2]

This work proposes a direct route for converting PET waste into a versatile platform of sustainable PEAs. An innovative series of PEAs was synthesised by bulk polycondensation of bis(2-hydroxyethyl) terephthalate (BHET), derived from PET glycolysis, and the bio-based monomer β-alanine. The molar ratio of the comonomers (BHET/β-alanine) was systematically adjusted from 90/10 to 10/90 in order to establish a fundamental parameter for modulating the final properties.

The structural confirmation of the copolymer architecture was carried out by FTIR and ^{1}H NMR spectroscopy. The thermal profile, analysed by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), revealed that key properties, such as glass transition temperature (T_g) and the onset of thermal decomposition, can be precisely modulated within the series, establishing a robust composition-property correlation. [3,4]

By successfully transforming a ubiquitous plastic waste stream into a family of polymers with tunable characteristics, this research opens a viable pathway to reducing dependence on virgin petrochemical resources. The investigated sustainable PEAs show potential for high value-added applications such as technical textiles requiring resistant fibres, bioactive scaffolds for tissue engineering, or barrier materials for packaging.[5]

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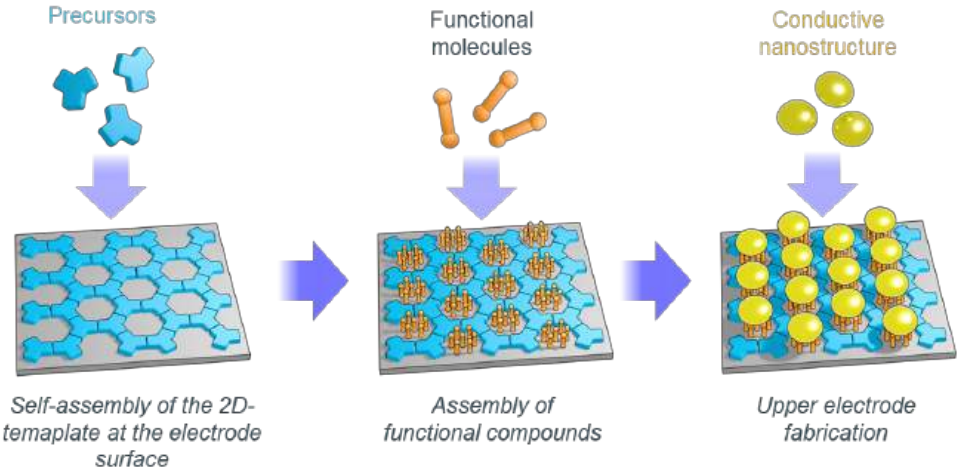
IM - D2 – P12
Molecular templates as platforms for controlled surface fabrication of molecular electronic devices

Enrique Escorihuela[1,2,3,4], Steven De Feyter[1], Pilar Cea[2,3,4]
[1]Dept. of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Belgium; [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-University of Zaragoza, Spain; [3]Physical Chemistry Dept. of the University of Zaragoza, Spain; [4]Laboratorio de Microscopias Avanzadas (LMA), University of Zaragoza, Spain

The use of molecules as electronic components has garnered significant attention since Aviram and Ratner conceived the idea in 1974. Over the past decades, numerous organic compounds have been studied and demonstrated to function as current rectifiers, resistors, switches, or transistors. However, achieving efficient and reliable electrical contacts to a large number of individual molecules remains one of the key challenges in Molecular Electronics, hindering the fabrication of functional devices.[1]
Herein, we present a compilation of template-based strategies to direct the integration of individual or a limited number of molecules into electronic devices on electrode surfaces. These approaches exploit either the spontaneous self-assembly of organic compounds into molecular networks, such as dehydrobenzoannulene or benzoic acid derivatives, or the use of the Langmuir-Blodgett technique to achieve controlled molecular packing. Therefore, the incorporation of functional electronic molecules by self-assembly or electrografting is governed by the electrode-template interface,[2] in which the molecular patterns either expose discrete regions of the electrode or serve as specific anchoring sites. Finally, the incorporation of the upper electrode, such as metallic nanoparticles, completes the circuit, enabling the measurement of the electrical properties of these systems by conductive scanning probe microscopies, including STM and conductive AFM.
This approach benefits from large-area fabrication techniques by sequentially combining different materials to produce discrete and isolated devices through a relatively straightforward methodology, enabling a high device yield per unit area and allowing modulation of device properties and arrangements based on the shape of the underlying pattern.



Scheme of the fabrication process of isolated molecular devices on the electrode surface.

This work was supported by KU Leuven–Internal Funds (C14/23/090) and the Odón de Buen Postdoctoral Grant from the Government of Aragón.

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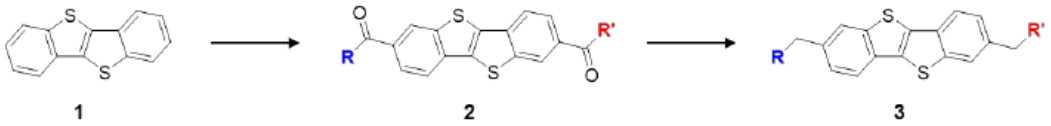
IM - D2 – P13
Greener synthetic strategies toward small-molecule organic semiconductors

Magdalena Steinbrugger[1], Suman Mallick[1], Thomas Rath[1], Gregor Trimmel[1]
[1]*Institute for Chemistry and Technology of Materials, Graz University of Technology, Austria*

Organic semiconductors based on fused heteroacene architectures are key materials in organic electronics. Among these systems, [1]benzothieno[3,2-b][1]benzothiophene (BTBT, **1**) and its derivatives are widely used as benchmark p-type organic semiconductors.[1] Despite their relevance, synthetic access to BTBT-based materials often relies on environmentally unfavorable protocols and solvent-intensive purification techniques.
In this work, alternative synthetic strategies toward functionalized BTBT derivatives are explored, with the aim of improving synthetic flexibility while considering more sustainable reaction pathways. An improved synthetic route to the BTBT core was established using a greener solvent system, replacing conventionally used solvents while maintaining reliable access to the target structure. Subsequent electrophilic aromatic substitution of the BTBT core enabled the preparation of a series of substituted derivatives, which were further modified to access structurally diverse compounds (Scheme 1).
Mechanochemical conditions were implemented as an alternative to conventional solution-based functionalization for Friedel-Crafts-type reactions on the BTBT core, enabling shorter reaction times while maintaining effective reactivity. In addition, one-pot approaches toward asymmetrically functionalized BTBT derivatives were investigated to reduce the need for sequential transformation steps.
Current work focuses on expanding the molecular library and investigating the influence of substitution patterns on processability and optoelectronic properties. Overall, this study contributes to more sustainable synthetic strategies toward BTBT-based organic semiconductors, providing a foundation for future materials studies relevant to organic electronics.



Scheme 1. Synthetic pathway for the functionalization of the BTBT core (**1**) via acylated intermediates (**2**), leading to symmetrically and asymmetrically substituted BTBT derivatives (**3**).

This work is supported by the European Innovation Council through the GreenOMorph project (Grant No. 101161637).

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IM - D2 – P14

Fabrication of robust films of electrochromic materials: Towards smart device applications

Dien Duy Nguyen[1], Thanh Hai Phan[2], Steven De Feyter[1]
[1]Division of Molecular Imaging and Photonics, Dept. of Chemistry, KU Leuven, Belgium; [2]Dept. of Physics and Materials Science, Faculty of Natural Sciences, Quy Nhon University, Vietnam

Electrochromic materials (ECMs) are functional materials that change color under an applied electric field, enabling applications in smart windows, displays, and energy-saving devices [1]. Among them, viologen derivatives are highly promising due to their high optical contrast, coloration efficiency, redox stability, and tunable molecular design[2,3]. However, practical deployment of viologen-based ECMs remains limited by poor cycling stability, uneven color performance, and structural disorder at the electrode interface, which hinders efficient charge transfer and long-term durability[4]. A promising strategy to overcome these challenges is the fabrication of robust electrochromic materials (RECMs) with controlled monolayer or nanopatterned architectures. Covalent grafting of viologen molecules onto conductive substrates stabilizes the electrochromic films and allows precise control over molecular ordering and thickness. Transparent and flexible electrodes such as indium tin oxide (ITO), together with atomically flat model substrates such as highly oriented pyrolytic graphite (HOPG), provide complementary platforms for device integration and molecular-resolution investigation. This research aims to develop reproducible electrochemical grafting protocols for g-dibenzyl viologen (g-DBV) and g-diphenyl viologen (g-DPV) on HOPG and ITO electrodes. The grafted layers will be characterized by scanning tunnelling microscopy (STM), atomic force microscopy (AFM), and Raman spectroscopy to provide molecular-scale insight into surface morphology, molecular ordering, and covalent attachment. By correlating nanoscale structures with electrochromic behavior, this work seeks to clarify structure–function relationships governing coloration efficiency, switching speed, and operational stability. Ultimately, the project targets lab-scale RECM devices with improved durability, fast response, tunable optical properties, contributing to next-generation flexible electrochromic technologies for smart device applications.

Acknowledgement: The authors gratefully acknowledge financial support from KU Leuven–Internal Funds (C1 C14/23/090), the Research Foundation – Flanders (FWO), Belgium (G0DAW23N) and National Foundation for Science and Technology Development (NAFOSTED), Vietnam - Project code: FWO.104-2022.03.

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IM - D2 – P15

Effect of PVA concentration on the morphology and characteristics of hydroxyapatite microspheres prepared by spray drying

Tae Joon Park[1, 2], Oak Sam Park[1, 2], Jun Seop Lee[3, 4], Dae Yong Jeong , Hye Sun[3*]
[1]Advanced Bio-Composite Lab, CM Biopharm Co., Ltd., Cheongju-si, Republic of Korea; [2]Dept. of Materials Science and Engineering, Inha University, Republic of Korea; [3]Bio-Convergence R&D Group, Korea Institute of Ceramic Engineering & Technology, Cheongju-si; Republic of Korea; [4]Dept. of Dental Biomaterials, Kyungpook National University, Republic of Korea

Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, HAp) has been extensively applied in biomedical and industrial fields owing to its excellent biocompatibility and chemical stability. In this study, the effect of precursor viscosity−modulated by the addition of a polymeric binder−on the morphology of spray-dried HAp microparticles was systematically investigated. Gel precursors with controlled viscosities were prepared and characterized rheologically to elucidate the correlation between viscosity and droplet formation behavior during atomization. The morphology and microstructure of the resultant particles were examined by SEM, XRD, and N_2 adsorption (BET) analyses. It was found that precursor viscosity critically governs particle sphericity and size uniformity: low viscosities resulted in collapsed or irregular morphologies, whereas excessively high viscosities impeded atomization. Within the optimal viscosity window of 800–900 mPa·s (at 1 s^{-1}), uniform and dense spherical HAp particles with an average diameter of approximately 40 μm were obtained. A mechanism describing viscosity-controlled morphological evolution is proposed, emphasizing the balance between solvent evaporation rate and droplet solidification kinetics. These findings provide practical guidance for the scalable production of flowable bioceramic microspheres.

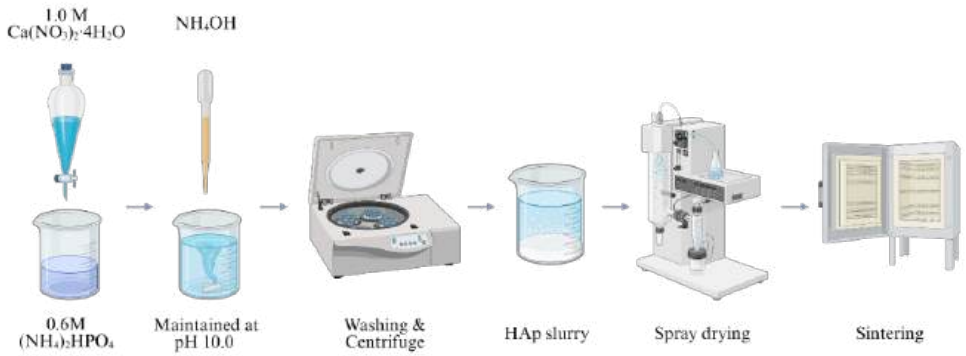

Figure 1. Schematic illustration of the hydroxyapatite (HAp) precipitation process, including reagent mixing, washing with ethanol, drying and sintering to obtain the final HAp powder.

This study was supported by a grant from the Korea Institute of Ceramic Engineering and Technology (KICET) [grant number: 2410013749]; the Government-wide R&D to Advance Infectious Disease Prevention and Control, Republic of Korea [grant number: RS-2023-KH14035]; This study was supported by the 2025 Bio-medicine Raw Materials Commercialization Support Program funded by the Bio-medicine Raw Materials Commercialization Support Business Group; and the 2025 Corporate Growth Support Program funded by the Chungbuk Bio Industry-Academy Convergence Institute.

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IM - D2 – P16
Upscaling the exfoliation process of montmorillonite for epoxy nanocomposites

Mark Joseph Mitra Pasciolco[1], Khianne Ed Miguel Orteza[1], John Loui Tadia[1], Wei Han[2], King Lun Yeung[1,2]
[1]Dept. of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, China; [2]Division of Environment and Sustainability, The Hong Kong University of Science and Technology, China

The use of coatings has been considered as the most economically efficient method to protect metallic surfaces like pipes from corrosion and biofouling. Epoxy itself is porous and hydrophilic, thus incorporation of fillers is an option to improve its mechanical and anticorrosion properties. In recent years, 2D nanomaterials like montmorillonite (MMT) are immensely studied as potential nanofillers for modified epoxy coatings. These nanomaterials need to be exfoliated to reduce the thickness of each particle, lessen the chance to agglomerate, and make the nanomaterial easier to be modified or functionalized. The current concern in this field is the upscaling of production of exfoliated nanomaterials as exfoliation studies in literature used small amount of feed, giving low yield which is a challenge in the mass production of epoxy nanocomposite coatings. This study aims to upscale the exfoliation process of MMT and compare their properties. Different amounts of montmorillonite (1, 3, and 5g) were used to determine if it will affect the quality of the exfoliated 2D nanomaterial. SEM images showed that there are no differences in surface morphology, and the FTIR spectra of the exfoliated nanomaterials from different batches are the same. Basal spacing from XRD is around 1.5nm for all samples. Lastly, AFM showed that the thickness of around 75-80 nm is observed for all batches. Thus, feeding more MMT in the exfoliation process will not just give higher yield, but it will also have the same properties with the nanomaterial exfoliated in smaller scale.

Keywords: exfoliation, montmorillonite, epoxy nanocomposite

IM - D2 – P17
Experimental investigation of hydrogen storage in defective fullerenes

Mehmet Doğan[1], Mehmet Yaşar Kalafat[1], Berna Koçer Kızılduman[1], Zeynep Bicil[1], Yasemin Turhan[1], Ersin Yanmaz[2], Betül Duman[1]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey; [2]Balikesir University, Altınoluk Vocational School, Dept. of Chemical and Chemical Processing Technologies, Turkey

Defective fullerenes have been extensively explored through theoretical and computational approaches for hydrogen storage; however, experimental validation remains highly limited. In this study, hydrogen storage in defective fullerenes is systematically investigated through direct experimental synthesis, comprehensive characterization, and adsorption measurements. Defective structures were generated from pristine C60 using high-energy mechanical milling under controlled grinding time and rate, enabling tailored structural modification.
Structural, spectroscopic, and morphological analyses demonstrated progressive disruption of the fullerene cage, accompanied by reduced particle size, altered surface topography, and partial amorphization. Thermal analysis revealed a transition from single-step decomposition in pristine fullerene to multi-step decomposition behavior in defective samples, confirming structural deformation. Surface area and pore characteristics showed non-monotonic variation with milling conditions; nevertheless, the sample prepared at 1 h and 500 rpm exhibited the highest BET surface area and micropore volume.
Hydrogen adsorption measurements were conducted at room and cryogenic temperatures over a wide pressure range. Defective fullerenes displayed enhanced hydrogen storage capacities compared to pristine C60, with the D-C60-1 h-500 rpm sample reaching a maximum uptake of 2.17 wt% at 97 bar. At ambient temperature, adsorption followed Henry-type behavior, while cryogenic measurements exhibited multilayer adsorption with pronounced hysteresis, consistent with Type IV isotherms and mesoporous characteristics. These results indicate that defect formation facilitates hydrogen access not only to external surfaces but also to the partially opened interior of the fullerene structure.
Kinetic analysis showed that hydrogen adsorption data were best described by the pseudo-second-order model, highlighting the dominant role of defect-induced adsorption sites. Overall, this work provides the first comprehensive experimental framework linking defect engineering in fullerenes to hydrogen storage performance, offering critical experimental insight to complement existing theoretical predictions.

The authors gratefully acknowledge the financial support of TÜBİTAK (The Scientific and Technological Research Council of Türkiye) under Project No. 123Z536.

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IM - D2 – P18
Lithium-induced defect design in fullerene structures for enhanced hydrogen storage

Mehmet Doğan[1], Yasemin Turhan[1], Betül Duman[1], Zeynep Bicil[1],Berna Koçer Kızılduman[1], Ersin Yanmaz[2]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey; [2]Balikesir University, Altınoluk Vocational School, Dept. of Chemical and Chemical Processing Technologies, Turkey

This work explores a defect-assisted lithium doping strategy to enhance the hydrogen storage performance of fullerene-based materials. Pristine C_{60} was structurally modified via high-energy ball milling to introduce lattice defects, followed by lithium incorporation through hydrothermal treatment. This sequential modification enabled simultaneous control of structural disorder and dopant distribution within the fullerene framework.
Fourier transform infrared spectroscopy confirmed the disruption of characteristic vibrational modes of pristine C_{60} and the appearance of new bands associated with defect formation and lithium–carbon interactions. Thermal analyses demonstrated that both defect generation and lithium incorporation modified the thermal stability and decomposition behavior of fullerene, indicating altered bonding environments and structural integrity. Scanning electron microscopy revealed pronounced morphological evolution, including particle fragmentation, surface roughening, and increased agglomeration in Li-doped defective samples, consistent with symmetry loss and enhanced surface heterogeneity induced by milling and doping.
Hydrogen adsorption measurements showed that storage capacity strongly depends on lithium concentration, processing temperature, and treatment duration. Among all samples, Li-doped defective fullerene synthesized using 0.1 M $LiNO_3$ at 200 °C for 12 h exhibited the highest hydrogen uptake under high-pressure conditions. This enhancement is attributed to the combined effects of increased accessible surface area and enlarged micropore volume. Adsorption isotherms were described by both Langmuir and Freundlich models, indicating heterogeneous surface energetics dominated by physisorption. Kinetic data followed a pseudo-second-order model, suggesting that intraparticle diffusion governs adsorption.
Electrochemical impedance spectroscopy revealed reduced charge-transfer resistance and enhanced conductivity in Li-doped samples, highlighting the role of lithium-induced electronic pathways in diffusion-assisted transport. Pearson correlation analysis demonstrated strong positive correlations between hydrogen storage capacity and both BET surface area and micropore volume, with surface area showing a stronger influence. Overall, the results demonstrate that lithium-induced defect engineering is an effective approach for tailoring fullerene-based materials toward efficient and reversible hydrogen storage applications.

The authors gratefully acknowledge the financial support of TÜBİTAK (The Scientific and Technological Research Council of Türkiye) under Project No. 123Z536.

IM - D2 – P19
MOF-5-based fullerene nanocomposites for enhanced hydrogen storage applications

Berna Koçer Kızılduman[1], Cemre Makbule Yıldız[1], Mehmet Doğan[1], Zeynep Bicil[1], Yasemin Turhan[1], Ersin Yanmaz[2]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey; [2]Balikesir University, Altınoluk Vocational School, Dept. of Chemical and Chemical Processing Technologies, Turkey

In this study, nanocomposites were synthesized using a metal–organic framework MOF-5 as the matrix and fullerene (C60) and defective fullerene (D-C60) as filler materials, and their hydrogen storage performances were systematically investigated. The nanocomposites were prepared via a solvent removal method by incorporating filler contents of 1, 2.5, and 5 wt% into the MOF-5 matrix. Structural characterization revealed that the presence of the filler phase significantly influenced the MOF-5 framework. FTIR analyses indicated modifications in the characteristic band intensities of MOF-5 and the formation of new functional groups, suggesting interfacial interactions between the matrix and filler materials. XRD results demonstrated that the crystalline structure of MOF-5 was largely preserved after filler incorporation, while variations in peak intensities and slight shifts in peak positions implied structural interactions and partial reductions in crystallinity. Thermogravimetric analysis showed that the thermal stability and decomposition behavior of MOF-5 were enhanced by the incorporation of both C60 and D-C60 SEM observations revealed that D-C60-filled nanocomposites exhibited a more homogeneous particle distribution and denser morphology compared to their C60-filled counterparts. BET surface area analyses confirmed that the nanocomposites possessed higher specific surface areas and micropore volumes relative to pristine MOF-5. Hydrogen adsorption isotherms demonstrated that the storage capacity strongly depended on filler type, filler content, temperature, and pressure. Isotherm modeling showed good agreement with Freundlich model, with high correlation coefficients, while kinetic studies indicated that the adsorption process followed a pseudo-second-order model governed by an intraparticle diffusion mechanism. Overall, the results highlight that fullerene- and defective fullerene-incorporated MOF-5 nanocomposites are promising candidate materials for advanced hydrogen storage applications.

Many thanks to the Scientific and Technological Research Council of Türkiye (TÜBİTAK) for supporting this study with project number 123Z536.

IM - D2 – P20

Functionalized carbon nanotube-based affinity matrices for efficient purification and kinetic evaluation of polyphenol oxidase

Mehmet Doğan[1], Fatma Nur Yalçınkaya[1], Serap Doğan[1], Zeynep Bicil[1], Pınar Turan Beyli[1], Berna Koçer Kızılduman[1], Şeyma Çam[1]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey

In this work, functionalized multi-walled carbon nanotubes (MWCNTs) were developed as affinity support materials for the purification and biochemical characterization of polyphenol oxidase (PPO) obtained from different biological sources. Surface modification of pristine MWCNTs was carried out to introduce functional groups capable of promoting specific enzyme–support interactions. Structural and textural changes induced by functionalization were systematically examined using complementary characterization techniques. A decrease in BET surface area from 278.0 to 202.8 $m^2 g^{-1}$ confirmed the successful grafting of functional moieties onto the nanotube surface, indicating partial pore blocking accompanied by enhanced surface chemistry.

The functionalized MWCNT-based affinity matrix demonstrated high purification efficiency for PPO isolated from Salvia officinalis L., Salvia aethiopis L., and mushroom extracts. Purification folds of 16.4, 8.4, and 12.9, respectively, were achieved under optimized chromatographic conditions. SDS-PAGE analysis of purified PPO from S. officinalis L. revealed a single dominant protein band with an estimated molecular weight of approximately 43–45 kDa, confirming high purity and structural integrity of the enzyme following isolation.

The biochemical properties of purified PPO were further investigated through activity assays conducted with different phenolic substrates. Optimum pH and temperature values varied depending on both the enzyme source and substrate type, highlighting substrate-specific catalytic behavior. Kinetic analyses showed that PPO exhibited distinct Michaelis–Menten parameters toward catechol, 4-methylcatechol, and pyrogallol. Among these substrates, pyrogallol displayed the highest catalytic efficiency, as reflected by its elevated Vmax/KM ratio, indicating stronger enzyme–substrate affinity and faster turnover.

Overall, the results demonstrate that functionalized MWCNTs serve as robust and reusable affinity supports for PPO purification while preserving enzymatic activity and catalytic performance. This approach offers a versatile platform for enzyme isolation and characterization, positioning both Salvia species and mushroom-derived PPO as valuable biocatalysts for industrial, analytical, and biotechnological applications.

The authors gratefully acknowledge the financial support of TÜBİTAK (The Scientific and Technological Research Council of Türkiye) under Project No. 122Z634.

IM - D2 – P21
Defect-dopant interactions in graphene-fullerene nanocomposites for hydrogen storage

Yasemin Turhan[1], Betül Duman[1], Mehmet Doğan[1], Ersin Yanmaz[2], Zeynep Bicil[1],Berna Koçer Kızılduman[1]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey; [2]Balikesir University, Altınoluk Vocational School, Dept. of Chemical and Chemical Processing Technologies, Turkey

This study discusses the role of defect-doping interaction of the reinforcing phase fullerene in developing high-performance hydrogen adsorbents of graphene-based nanocomposites. Pure C60 was milled and transformed into defective C60 (D-C60) and Li-doped defective C60 (Li-D-C60), respectively, and then graphene was incorporated in various ratios to form defect-rich hybrid architectures. Morphological analyses revealed Type IV adsorption isotherms with combined micro-mesopoility, while kinetic modeling confirmed pseudo second-order behavior ($R^2 > 0.99$) consistent with Langmuir monolayer adsorption ($R^2 \approx 0.996$). The optimized Graphene-P2.5-Li-D-C60 sample achieved a hydrogen storage capacity of 2.53% at 77 K and 100 bar, surpassing the capacities of pure graphene (1.81%) and D-C60 (2.17%). Mechanistic analyses revealed a multi-step adsorption mechanism where boundary layer diffusion predominates in the initial phase and intraparticle diffusion as equilibrium is approached. This stepwise process, coupled with defect-induced active site enrichment and Li-driven surface polarization, enhanced both hydrogen accessibility and binding strength. Pearson correlation analysis ($r = 0.50$ for BET surface area and $r = 0.51$ for micropore volume) demonstrated that hydrogen storage performance is not solely governed by textural properties but stems from a synergistic interaction between porosity, diffusion kinetics, and electronic polarization effects. These findings reveal the structure-diffusion-polarization coupling mechanism and demonstrate the hydrogen storage potential of these nanocomposites for efficient and reversible cryogenic hydrogen storage.

The authors gratefully acknowledge the financial support of TÜBİTAK (The Scientific and Technological Research Council of Türkiye) under Project No. 123Z536.

IM - D2 – P22

Hydrothermal titanium doping of defect-engineered fullerenes for enhanced hydrogen storage

Şeyma ÇAM[1], Mehmet Doğan[1], Zeynep Bicil[1], Berna Koçer Kızılduman[1], Yasemin Turhan[1], Ersin Yanmaz[2]
[1]Balikesir University, Faculty of Science and Literature, Dept. of Chemistry, Turkey; [2]Balikesir University, Altınoluk Vocational School, Dept. of Chemical and Chemical Processing Technologies, Turkey

Defect-engineered fullerenes (D-C60) obtained by high-energy ball milling were hydrothermally doped with titanium using an ammonium hexafluorotitanate precursor. The influence of dopant concentration, reaction temperature and reaction time was systematically investigated to optimize structural and adsorption properties. Structural evolution was examined by FTIR, XRD, SEM/EDX, TG, BET surface area and pore volume analyses.

FTIR spectra confirmed the presence of oxygen-containing defect sites and indicated strong interaction between titanium species and surface functional groups. XRD patterns exhibited broad diffraction features characteristic of partially disordered carbon structures, and increased structural distortion was observed under more severe reaction conditions. SEM images revealed noticeable changes in particle morphology after titanium incorporation, showing a more heterogeneous and textured surface consistent with dopant-induced modification. EDX verified successful titanium incorporation, increasing with precursor concentration.

Textural analysis demonstrated that controlled doping enhanced surface development and microporosity, while excessive reaction severity promoted partial pore collapse and reduced thermal stability. Moderate hydrothermal parameters provided the most favorable balance between dopant incorporation and structural integrity.

Hydrogen adsorption measurements up to 105 bar demonstrated that a titanium-doped defective fullerene sample achieved the highest uptake of 2.20 wt%, indicating that optimized titanium incorporation enhances hydrogen storage performance. Variations in concentration, temperature and reaction time significantly influenced adsorption behavior, highlighting the strong sensitivity of hydrogen uptake to defect–dopant interaction. Overall, the results demonstrate that controlled hydrothermal titanium doping of defect-engineered fullerenes provides an effective strategy for improving hydrogen storage through tailored surface and structural modification.

The authors gratefully acknowledge the financial support of TÜBİTAK (The Scientific and Technological Research Council of Türkiye) under Project No. 123Z536.

IM - D2 – P23
A linear carbazole-based phosphonic acid for enhanced efficiency in 3D perovskite solar cells

Robin Erkens[1], Wouter Van Gompel[1]
[1]Hasselt University, Institute for Materials Research in Microelectronic (IMO-IMOMEC), Hybrid material Design (HyMaD), Belgium

Self-assembled monolayers (SAMs) of phosphonic acids play a critical role as hole-selective contacts in high-efficiency inverted (p–i–n) perovskite solar cells. The widely used benchmark molecule, 2PACz, is itself carbazole-based and has enabled state-of-the-art device performance; however, its non-linear molecular geometry can impose limitations on monolayer packing and interfacial order. In this work, we report a new linear carbazole-based phosphonic acid designed to improve interfacial properties through a more extended molecular architecture.
The linear geometry of the phosphonic acid promotes improved ordering and surface coverage on transparent conducting oxides, leading to more favorable conditions for subsequent three-dimensional (3D) perovskite film formation. Perovskite solar cells incorporating this new SAM consistently outperform reference devices based on 2PACz, exhibiting higher power conversion efficiencies. The performance enhancement is primarily driven by improvements in open-circuit voltage and fill factor, indicating more efficient charge extraction and reduced interfacial losses at the buried contact.
These results demonstrate that even within the well-established class of carbazole-based phosphonic acids, targeted molecular redesign can yield meaningful gains in device performance. The introduction of a linear carbazole phosphonic acid provides a straightforward and effective strategy to surpass the efficiency of 2PACz in 3D perovskite solar cells, highlighting the continued potential of interfacial molecular engineering for advancing perovskite photovoltaic technologies.

Research was funded by the FWO (1SB3725N)

IM - D2 – P24

ETS-10 coated honeycombs as possible candidate for CO_2 capture in humid flue gas streams

Morgane Van Hove[1,2], Ben Sutens[1], Steven Mullens[1], Guy De Weireld[2]
[1]Flemish Institute for Technological Research (VITO NV), Belgium; [2]University of Mons, Faculty of Engineering (UMONS), Belgium

To limit global warming to below 1.5°C, net-zero CO_2 emissions must be achieved by 2050. While reduction of energy consumption and transitioning to renewable energy are essential, it has an insufficient impact in a short-term and worldwide scale.[1] Carbon dioxide removal strategies such as Carbon Capture Utilisation and Storage (CCUS) are therefore critical especially in hard-to-abate sectors.[2] Current industrial CCUS relies on liquid amine absorption, which suffers from high energy demand and solvent degradation.[3] Solid adsorbents offer a promising alternative, yet their CO_2 capacity in humid conditions remains a major challenge.[4]
ETS-10, a titanosilicate zeolite, has shown that it retains its CO_2 uptake under high relative humidity (90% RH) in powder form.[5] However, whether this moisture tolerance is preserved in structured configurations remains unclear. Given its production on kg scale, ETS-10 was selected for structuring on cordierite honeycombs via vacuum wash-coating to assess its dynamic performance under realistic flue gas conditions. Initial characterisation (XRD, SEM-EDX, TGA-MS, N_2 sorption) confirmed material purity and porosity. Firstly, static CO_2 and H_2O isotherms were measured, then dynamic breakthrough experiments revealed more insights in mixed streams. ETS-10 structured on honeycombs demonstrated promising CO_2 uptake under humid conditions, suggesting potential for outperforming conventional zeolites when integration precedes H_2O displacement. However, precise capacity values and direct comparisons remain under investigation due to differences in humidity levels and measurement conditions.[6]
To further reduce moisture effect, cation exchange was explored. Inspired by studies on 13X, Na-ETS-10 was exchanged with H^+, K^+, Ba^{2+}, and Cs^+. Among these, K-ETS-10 exhibited the best balance in retaining CO_2 capacity while reducing H_2O uptake. Protocols to improve K^+ exchange degree were implemented, enabling the production of optimized ETS-10 on a large scale. The material was successfully structured on honeycombs and benchmarked against Na-ETS-10 to evaluate its dynamic performance.
These findings highlight ETS-10's potential as a moisture-insensitive adsorbent for CO_2 capture in humid flue gas streams, offering a scalable and energy-efficient alternative to conventional technologies.

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IM - D3 - P01
Multifunctional degradable titanium coatings for osteointegrative and antimicrobial surfaces

Mariana Busila[1], Cosmin Romanitan[2], Oana Brincoveanu[2], Vasilica Tucureanu[2], Alina-Mihaela Cantaragiu Ceoromila[3], Aurel Tabacaru[4] and Violeta Dediu[2]
[1]Interdisciplinary Research Center in the field of Eco-Nano Technology and Innovative Materials (CC-ITI), Faculty of Engineering, Dunarea de Jos University of Galati, Romania; [2]National Research and Development Institute in Microtechnologies – IMT Bucharest, Romania; [3]Dept. of Applied Sciences, Cross-Border Faculty, "Dunarea de Jos" University of Galati, Romania; [4]Dept. of Applied Sciences, Sciences and Environment Faculty, "Dunarea de Jos" University of Galati, Romania

The rational design of multifunctional surface coatings for titanium implants requires precise control over composition, interfacial chemistry, and degradation behavior in biologically relevant environments. Recent advances in hybrid materials chemistry emphasize the importance of combining organic and inorganic building blocks to achieve synergistic functionality through controlled interfacial interactions [1-3]. In this contribution, we report a degradable hybrid composite coating deposited on titanium substrates via a dip-coating strategy, integrating biopolymeric and mineral phases to achieve enhanced bioactivity and antimicrobial performance.
The coating system is based on a multilayer composite architecture that combines collagen and nano-hydroxyapatite (nHA) as an inner bioactive phase with an outer chitosan-based biodegradable matrix incorporating gold-doped zinc oxide quantum dots (ZnO: Au QDs) and nystatin [4,5]. From a chemical standpoint, collagen and nHA form a hybrid interface stabilized by hydrogen bonding, electrostatic interactions, and calcium–phosphate coordination, closely resembling mineralized extracellular matrices. Chitosan provides a cationic polymer network capable of interacting with both the hybrid layer and the embedded functional species through non-covalent interactions, including ionic pairing and hydrogen bonding. These interactions play a key role in controlling coating cohesion, stability, and degradation behavior [6].
The dip-coating approach enables precise control over layer composition and thickness, while crosslinking reactions ensure sufficient coating integrity without compromising biodegradability. Chemical and structural characterization using complementary spectroscopic and microscopic techniques provides insight into hybrid interfacial interactions, which govern coating stability, degradation kinetics, and the release behavior of active components. The degradable nature of the composite allows gradual exposure of the bioactive phase and controlled release of antimicrobial and antifungal agents, primarily driven by matrix erosion and interfacial chemistry rather than bulk dissolution.
Overall, this work highlights how rational hybrid materials chemistry enables the design of advanced multifunctional coatings that bridge fundamental interface engineering with application-driven requirements for next-generation titanium-based implant surfaces.

Acknowledgements: This work was supported by the Scientific Research contract no. RF 828 dated 11.12.2024, in partnership with SC ARTZ Dent SRL, Galati, Romania, within the project entitled "Development of Functional Surfaces for Dental Implants: Hydroxyapatite Enriched with Bioactive Agents for Osseointegration and Antimicrobial Protection", Acronym BIOHAF (Biocompatible Implants Optimized with Hydroxyapatite and Functional Additives).

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IM - D3 - P02

Development of 2D nanosheets of lanthanide-based metal organic frameworks for developing a super-hydrophilic and super-oleophobic (underwater) selective layer on a ceramic support for separation of surfactant-stabilized oil-in-water emulsion

Abdul Waheed[1], Umair Baig[1]
[1]Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia

The current study aimed to develop an active layer composed solely of metal-organic frameworks for the efficient separation of oil-in-water emulsions. This was achieved by in situ growth of 2D nanosheets of a Ln-based metal-organic framework via solvothermal synthesis on a ceramic alumina disc. As a result, a continuous, defect-free active layer was formed on the ceramic alumina support. The resultant membrane, named as Ln-5-NH_2-IPA MOF, was studied for the separation of oil-in-water emulsion. The ultimate goal of the current study was to reduce the time and temperature required to synthesize 2D MOF sheets with a stable, active layer that can be tested under crossflow filtration conditions. The thickness of the 2D MOF nanosheets was found to be 1.8 nm on average, as observed in transmission electron microscopy. The *in-situ* growth of the 2D MOFs resulted in a dense coating on the ceramic support, resembling the leaves of densely growing trees in a forest. Owing to the dense growth of the 2D MOF on the ceramic support, the Ln-5-NH_2-IPA MOF membrane showed a high separation efficiency of >99% for the surfactant-stabilized 100 ppm crude oil-in-water emulsion during separation studies. Moreover, the membranes showed a permeance of 147.9 L m^{-2} h^{-1} bar^{-1} while using a crude oil-in-water emulsion. The membrane maintained stable performance, especially in separation efficiency, for 660 minutes, whereas its performance declined, with the normalized flux decreasing to 0.20 over 360 minutes. However, the membrane regained its flux following the cleaning cycle.

The authors are highly grateful for the support provided for conducting the current study. The current study was conducted at the Interdisciplinary Research Center for Membranes and Water Security at King Fahd University of Petroleum and Minerals, KSA.

IM - D3 - P03

Development of spherical Mg-Al silicate composites for simplified purification and enhanced filtration of C.A.S.E. polyols

Seungyun Han[1], Donghyun Kim[1], Jinkyu Kang[1], Dongmin Seong[1], Jaehun Jo[1]
[1]Giant Chemical, Korea South

Conventional sequential purification using magnesium and aluminum silicates for C.A.S.E. polyols is often challenged by process complexity and limited filtration efficiency. To address these limitations, this study developed a spherical Mg-Al silicate composite enabling a simplified, single-step purification process.

The optimized composite exhibited an average particle size of 94.60 ㎛ and a specific surface area of 514.51 m^2/g. Upon applying polyol purification, it achieved a 33.33% reduction in the CPR (reaching 30), thereby markedly improving reaction stability, while simultaneously decreasing filtration time by 52.66% (to 71 s).
These results demonstrate that the developed Mg-Al silicate composite substantially enhances overall process efficiency and offers a promising approach for the simplification and potential automation of high-purity polyol production.

IM - D3 - P04
Ultrathin macroporous substrates for near-field microscopy on free-standing membranes

Jenrik Bergjan[1], A.C. Basaran[1], Ö.D. Asik, A. Möller[1], K. Cosentino[2], W. Harneit,[1] M. Steinhart[1]
[1]Osnabrück University, Germany; [2]University Modena, Italy

Pore-spanning membranes (PSMs) are unsupported membrane segments suspended over a macroporous substrate for investigating the physical and functional properties of lipid bilayers under well-controlled conditions [1, 2, 3]. Conventional PSMs are typically optimized for far-field fluorescence microscopy, which limits spatial resolution and signal quality [4]. Integrating the PSM concept with advanced imaging techniques, such as optical super-resolution or near-field microscopy, has remained challenging. To this end, smooth macroporous substrates with nanoscale thickness and adequate mechanical stability are required. The macropores should have diameters of a few hundred nanometers, while the interpore spacing must be sufficiently large to allow individual macropores to be addressed by diffraction-limited microscopy and to enable the tethering of membranes on the macroporous substrates. Here, we report the use of porous alumina anodized with etidronic acid solutions [4] as a template for the fabrication of ultrathin macroporous gold foils that meet these stringent requirements. The undersides of the alumina templates were exposed by wet etching, followed by reactive ion etching to open the alumina pore bottoms. This procedure yielded a smooth macroporous surface suitable for gold deposition. After non-destructive detachment, unsupported ultrathin gold foils—containing holes corresponding to the initial alumina pore positions—were obtained and subsequently transferred onto microscope slides. By fine-tuning pore diameters and interpore spacing, lipid membranes can be suspended over the macroporous openings, ensuring minimal background, efficient signal transmission, and compatibility with high-intensity illumination. Our goal is to integrate PSMs with state-of-the-art super-resolution and near-field microscopy techniques, thus enabling nanoscale investigations of membrane organization and dynamics in unsupported membrane segments.

The authors thank the German Research Foundation for funding (RTG 2900: nanomaterials@biomembranes: Rationally designed surface architectures for nanoscale interrogation and manipulation of biomolecules at membranes, project number 501879556 and RIE/ICP Ion etching tool, project number 431858429).

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IM - D3 - P05
Carbon dots from renewable biomass precursors: Processing parameters and optical response

Rut Sisó-Moliné, Maria Cinta Pujol, Joan Josep Carvajal
Universitat Rovira i Virgili (URV), Departament de Química Física i Inorgànica, Spain

Biomass-derived carbon dots (CDs) constitute a heterogeneous family of nanostructured materials whose optical properties depend strongly on precursor composition and processing conditions[1,2]. This contribution addressed the preparation of CDs by bottom-up methods from selected waste streams, specifically hemicellulose and lignin from commercial sources and from residues such as almond shells and pig dry manure. The diversity of these feedstocks provided a basis for examining how the chemical composition influenced the characteristics of the resulting particles.
CDs were prepared by hydrothermal synthesis, and several experimental parameters were explored, including the pre-treatment of raw materials, the choice of solvent system, reaction temperature and duration, precursor concentration, and the application of simple pretreatments to the raw biomass. The objective was to determine how these variables affected the formation process and the optical response of the products. Standard physicochemical characterization techniques were employed to obtain information on particle size, surface properties, and functionality, as well as photoluminescence features.
As a potential application, the response of the synthesised CDs to temperature was examined to assess their suitability as luminescent probes. Changes in emission intensity and spectral profile under controlled heating–cooling cycles were used as preliminary indicators of sensitivity and reversibility. The work sought to contribute experimental information on the conversion of heterogeneous biogenic precursors into carbon-based nanomaterials and on the practical constraints associated with their reproducible preparation.

These results were supported by grants PID2021-128090OB-C22 funded by MICIU/AEI/10.13039/501100011033/ and FEDER/UE. Additional funding was provided by URV and Diputació de Tarragona through grant 2023PMF-PIPF-24.

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IM - D3 - P06
Imination of aminocaprolactam with bio-based aldehydes to produce bio-based polyamides

Runa Tschekorsky Orloff[1], Regina Palkovits[12]
[1]Institute of Technical and Macromolecular Chemistry (ITMC), RWTH Aachen University, Germany; [2]Institute for a Sustainable Hydrogen Economy, (INW-2), Forschungszentrum Jülich, Germany

A significant part of the development of modern society has relied on the use of fossil resources, both in the past and present. However, the growing global demand for carbon-based materials cannot be met by these finite reserves. Consequently, biomass has evolved as an important renewable carbon source and moved in the focus of current research. Trough the fermentation of sugars, the amino acid lysine can be produced in large quantities. Owing to its multifunctionality, featuring one carboxylic acid group, as well as two amino groups, lysine represents a promising bio-based platform chemical for the synthesis of value-added products.[1] The natural occurring homopolymer of lysine, ε-polylysine, is produced through fermentation but is limited to a low molecular weight range. Accessing high molecular weight ε-polylysine therefore requires a chemical approach. Conventionally, this involves cyclisation of lysine, protection of the α-amino group, polymerisation, and subsequent deprotection. Eliminating the protection step would significantly enhance the efficiency and sustainability of the process.[2]
The aim of this study was to develop bio-based monomers suitable for the production of ε-polylysine, while avoiding the protection step. Therefore, methylvanillin was employed as a bio-based aldehyde to form an imine with cyclised lysine. The reaction was carried out in methanol without the use of any additives. Reaction conditions were optimised with respect to temperature, time, concentration and aldehyde excess using a Bayesian optimisation. Highly selective conditions were identified, resulting in an imine yield of 91%. Furthermore, the substrate scope was extended to six additional bio-based aldehydes. In all cases, yields between 80 and 90% were achieved, demonstrating the robustness and versatility of the developed approach.

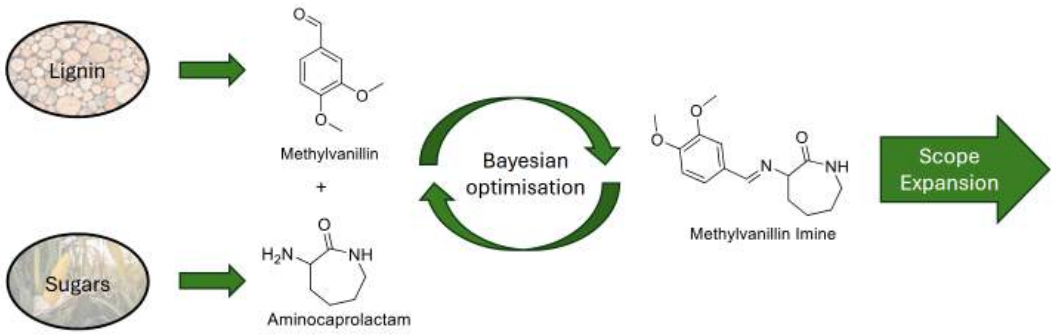

Fig. 1. Bayesian optimisation of aminocaprolactam imination and substrate scope.

This work was funded by the Werner Siemens Foundation in the frame of the WSS Research Centre "catalaix".

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IM - D3 - P07

Polymerization of malononitrile dimer: A new route for construction of nitrogen-rich polytriazines with functional properties

Juan Francisco Ruiz-Guerrón[1], Marta Ruiz-Bermejo[2], José Luis de la Fuente[1]
[1]Instituto Nacional de Técnica Aeroespacial "Esteban Terradas" (INTA), Spain; [2]Centro de Astrobiología (CAB) CSIC-INTA, Spain.

The search for new polymerization paths is an inevitable challenge in materials science, mainly with the advantages of simple operation, mild conditions, high efficiency, low cost, environmental benefits, reliability, and scalability. After many decades of exploring the chemistry of the C-C double bond, recently polymerizations based on triple bond building blocks have taken a clear lead role. Remarkable progress has been made in those where alkynes are used, however nitrile monomers have been less studied.
In this context, the thermally induced polymerization of amino-nitrile monomers, like the diaminomaleonitrile (DAMN), is becoming a valuable alternative to conventional polymerization methods, meeting the requirements argued above. Substantial advancements have been conducted by our group, starting with research on DAMN, which has been successfully polymerized thermally, both in solution and in bulk, yielding materials with interesting optoelectronic properties and promising applications.[1,2] In this same line, we have also focused on the bulk liquid thermal polymerization of aminomalononitrile.[3] The easy, quick, and highly efficient polymerization of these dinitrile compounds motivated the exploration of new multinitrile monomers, such as the malononitrile dimer, 2-amino-1,1,3-tricyanopropene (ATCP). Thus, a recent work revealed ATCP as a promising amino-nitrile monomer for the straightforward, one-pot synthesis of C=N conjugated organic materials featuring triazine linkages. DSC confirmed the successful bulk polymerization of ATCP, which proceeds upon melting and is initiated at relatively low temperatures without the need for solvents, catalysts, or initiators. The kinetic study carried out demonstrated the autocatalytic character and corroborated that these thermally induced reactions are extremely fast in a molten state. In addition, a preliminary structural characterization by spectroscopy supported the formation of triazine-based polymeric networks.[4]
These precedents encouraged us to explore the bulk thermal polymerization of ATCP at the preparative scale, and the structural characteristics of these ATCP-based polymers and their properties are discussed.

This research has been funded by grant Nº. PID2022-140180OB-C22 by the Spanish Ministry of Science and Innovation/State Agency of Research MCIN/AEI/ 10.13039/501100011033 and by "ERDF A way of making Europe". J. F. R.-G. thanks to INTA for his predoctoral contract.

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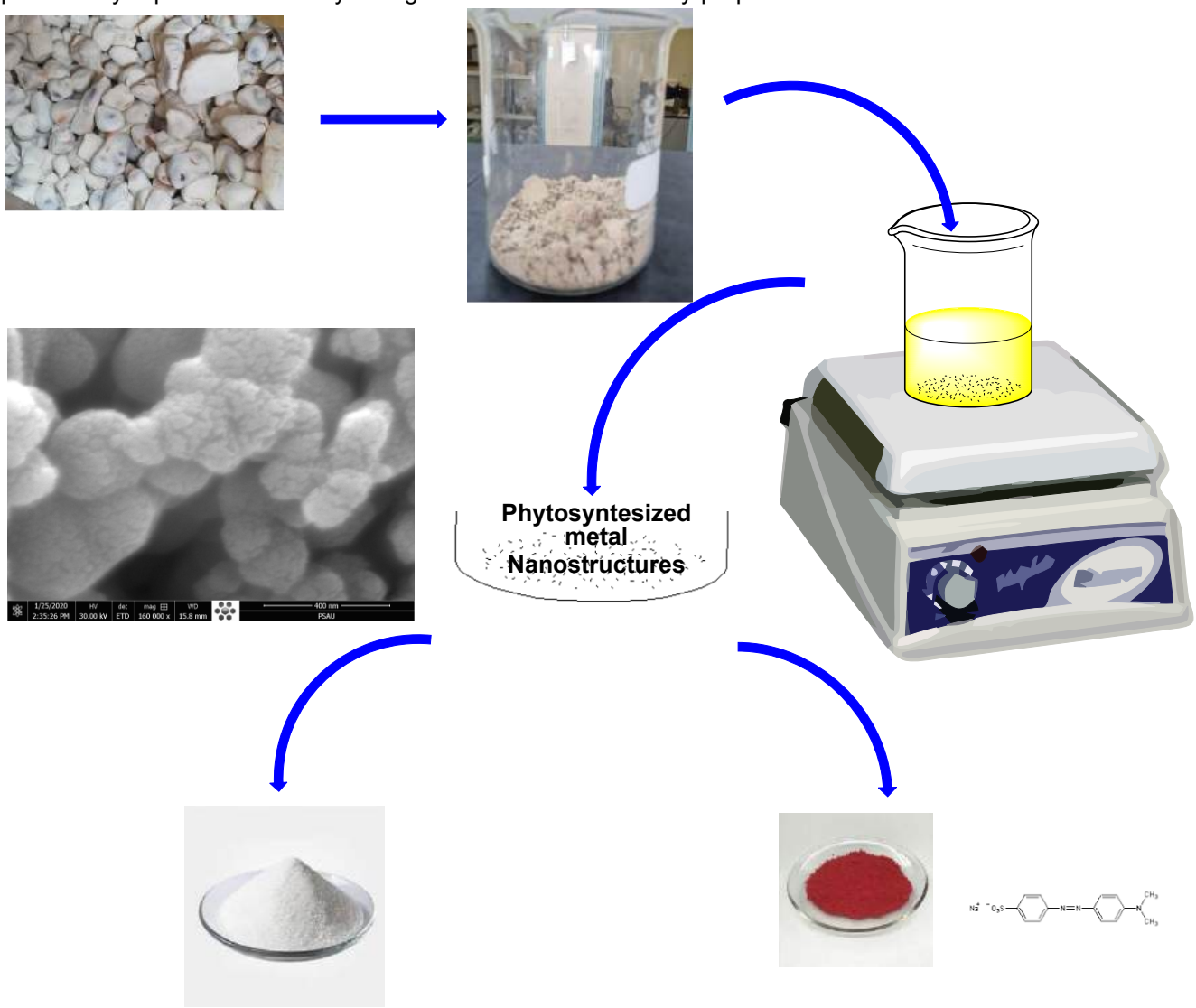
IM - D3 - P08

Biogenic synthesis of zinc oxide nanostructures using Adansonia digitata peel extract for sildenafil degradation and photocatalytic performance

Mohammed H. Geesi*[1], Oussama Ouerghi[2], Yassine Riadi[3]

[1]Dept. of Chemistry, College of science and humanities in Al-Kharj, Prince Sattam bin Abdulaziz University, Al-Kharj, Saudi Arabia; [2]Dept. of Physics, College of science and humanities in Al-Kharj, Prince; Sattam bin Abdulaziz University, Al-Kharj, Saudi Arabia; [3]Dept. of Medicinal Chemistry, College of Pharmacy, Prince Sattam bin Abdulaziz University, Al-Kharj, Saudi Arabia

Adansonia digitata plant usually used as source of food in many African countries. it contains many active compounds. In addition, its leaves and fruit extract was used as green source to prepare versatile metallic nanoparticles.[1] *Adansonia digitata* peel have been selected as a green route to the preparation of stable and shape-controlled zinc oxide nanostructures. Herein, an ecofriendly process based on using the water extract of *Adansonia digitata* peel to synthesize of ZnO nanoparticles[2]. The characterization of calcined zinc nanostructures, were performed using various physicochemical technics such as, Fourier-transform infrared spectroscopy, Raman, x-ray diffraction, Scanning electron microscope and X-ray photoelectron spectroscopy. Analytical characterisation technics used confirm the preparation of the targeted stable nanostructure. The photocatalytic sildenafil degradation of the green synthesized metal (Zn) nanostructures was assessed. Overall, the prepared zinc nanoparticles showed good efficacy towards degradation of tested drug. In addition, photocatalytic performance of dyes degradation of the ecofriendly-prepared nanostructures was also tested[3,4].



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IM - D3 - P09
Self-assembly of an amphiphilic copolymer and its potential as drug delivery systems

Ayşegül Özbal[1], Vural Bütün[1]
[1]Eskisehir Osmangazi University, Turkey

The design of advanced drug delivery systems has gained increasing interest in recent years in order to achieve the safe, efficient, and dose-controlled delivery of therapeutic agents to their intended targets. Among these systems, polymeric micelles derived from amphiphilic block copolymers have emerged as attractive carriers due to their ability to solubilize poorly water-soluble drugs and to provide controlled and prolonged release behaviors [1,2].
In the current study, a novel amphiphilic block copolymer, poly[(ethylene glycol) methyl ether methacrylate]-*b*-poly[(glycerol carbonate methacrylate)-*co*-(diisopropylamino)ethyl methacrylate] (PEGMEMA-*b*-P(GCMA-*co*-DPA)), was synthesized using reversible addition–fragmentation chain-transfer polymerization. The chemical composition and molecular characteristics of the copolymer were determined with ^{1}H NMR spectroscopy and gel permeation chromatography. At pH 7.4, the copolymer spontaneously self-assembled into polymeric micelles with an average hydrodynamic diameter of 20.1 nm. The structural features and morphology of the micelles were further investigated by ^{1}H NMR spectroscopy and transmission electron microscopy. Dipyridamole was employed as a model hydrophobic drug and efficiently encapsulated within the micellar core. The encapsulation efficiency and drug loading capacity of the micelles were quantitatively evaluated by UV–Vis spectroscopy.
In vitro drug release experiments conducted at pH 7.4 demonstrated controlled release profile. Overall, the findings indicate that PEGMEMA-*b*-P(GCMA-*co*-DPA) micelles represent a promising and adaptable carrier system for the delivery of hydrophobic therapeutic agents.

The authors gratefully acknowledge the financial support provided by Scientific and Technological Research Council of Türkiye (GN: 123C505)

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IM - D3 – P10
Design of new PEG-silanized fillers inspired by talc-like structures

Liva Dzene[1], Anne-Sophie Schuller[2], Séverinne Rigolet[1], Jocelyne Brendlé[1], Christelle Delaite[2]
[1]Institut de Science des Matériaux de Mulhouse CNRS UMR 7361, Université de Haute-Alsace, France; [2]Laboratoire de Photochimie et d'Ingénierie Macromoléculaires - EA4567, Université de Haute Alsace, France

Polymer–clay composites are well known for their enhanced mechanical and thermal properties, provided that the inorganic filler is homogeneously dispersed within the polymer matrix. Achieving such dispersion, however, remains challenging, particularly due to limited compatibility between polymers and pre-formed clay minerals. In this work, we investigate a fundamentally different approach, consisting of generating clay-like fillers in situ using silanized polymers as the silicon source. Beyond improving interfacial compatibility, this strategy also avoids the direct handling of nanoparticles, thereby reducing potential health risks.
Poly(ethylene glycol) methyl ether (mPEG) was functionalized with (3-isocyanatopropyl)triethoxysilane, yielding silane-terminated polymers with high functionalization efficiencies, exceeding 90%. These precursors were reacted with magnesium nitrate in ethanolic solution under basic conditions. mPEGs with molar masses ranging from 350 to 1900 g mol^{-1} were investigated, both alone and in combination with conventional silicon sources, tetraethyl orthosilicate and (3-aminopropyl)triethoxysilane.
When functionalized mPEG was used as the sole silicon source, the synthesis yields remained low, between 8 and 22 wt%. In contrast, combining functionalized mPEG with tetra or trialkoxysilane led to a threefold increase in yield, indicating enhanced network formation. Structural characterization by X-ray diffraction and FTIR spectroscopy revealed the formation of layered crystalline materials containing both Si–O and Mg–O bonds. However, solid-state 1H–29Si CPMAS NMR showed that silicon condensation was incomplete, with silicon predominantly present in T1 and T2 environments. SEM-EDX analysis further revealed Mg/Si molar ratios exceeding that of ideal talc.
Taken together, these results indicate that the synthesized materials more closely resemble functionalized brucite-like sheets rather than true talc analogues.[1] Nonetheless, this work establishes a viable route toward the in situ formation of layered organic–inorganic hybrids and provides a promising basis for the development of polymer–clay nanocomposites with improved filler dispersion

Acknowledgements: Laure Michelin, Ludovic Josien, and Habiba Nouali are acknowledged for their contributions to sample characterization. The study was funded via the project "Champs de recherche 2020" and "Recherche de l'UHA 2024" of the University of Haute-Alsace.

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IM - D3 – P11

Mass spectrometry–driven evaluation of antioxidant thermoplastic polyurethane films for waste cooking oil storage

Maria Assunta Acquavia[1,2], José J. Benítez[3], Susana Guzmán-Puyol[4], Patrizia Iannece[5], Carmine Gaeta[5], Giuliana Bianco[2], José A. Heredia-Guerrero[4]

[1]Istituto Nazionale di Ricerca Metrologica, MT; [2]Università degli Studi della Basilicata, Dipartimento di Scienze di Base e Applicate, Italy; [3]Insituto de Ciencia de Materiales de Sevilla, Centro Mixto CSIC-Universidad de Sevilla, Spain; [4]Instituto de Hortofruticultura Subtropical y Mediterránea La Mayora, Consejo Superior de Investigaciones Científicas-Universidad de Málaga- (IHSM, CSIC-UMA), Spain; [5]Università degli Studi di Salerno, Dipartimento di Chimica e Biologia, Italy

The stabilization and valorization of waste cooking oil (WCO) rely on storage solutions that can slow down oxidation and preserve the oil quality over time [1,2]. In this work, thermoplastic polyurethane (TPU) films containing α-tocopherol were developed as active materials for WCO storage. Their performances were evaluated using a combination of physicochemical and mass spectrometry-based analysis.

α-Tocopherol was selected as an active component as it combines strong antioxidant activity with a high affinity for lipid-rich systems, making it particularly suitable for interaction with waste cooking oil. TPU films with α-tocopherol between 5 and 20 wt% were prepared and characterized in terms of optical, thermal, mechanical, and barrier properties. The addition of the antioxidant improved UV protection, increased film flexibility, and reduced water vapor permeability, while preserving the mechanical strength and thermal stability required for real storage conditions.

Mass spectrometry played a central role in understanding how these materials work. LC–ESI–MS/MS was used to follow the controlled release of α-tocopherol into a lipid simulant, showing a sustained diffusion over time. Surface-sensitive analyses further indicated that the active compound can migrate to and from the film surface without causing polymer degradation.

To assess real performance, waste cooking oil was stored in contact with the TPU films and its chemical stability was monitored over time. MALDI–MS allowed direct molecular profiling of triacylglycerols, revealing that oils stored with TPU–α-tocopherol films retained a molecular composition closer to that of fresh oil after 90 days. In contrast, untreated samples showed clear signs of oxidation and degradation.

Overall, this study shows that TPU films incorporating α-tocopherol offer an effective and practical solution for extending the stability of waste cooking oil. The consistent use of mass spectrometry throughout the study highlights its value as a powerful tool for linking material design to molecular-level performance.

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IM - D3 – P12

A multifunctional nitrogen-doped magnetic graphene oxide nanocomposite prepared by one-step microwave-assisted synthesis

Émerson Leandro-Silva[1], Luiz Carlos Silva-Filho[1], Marina Piacenti-Silva[1]
[1]School of Sciences, Unesp, Brazil

This work reports the synthesis and characterization of a multifunctional nanocomposite based on magnetite-functionalized graphene oxide (mNGO), obtained through a one-step microwave-assisted hydrothermal route. The proposed strategy was designed to provide a rapid and controllable method for producing hybrid materials with integrated magnetic and photoactive properties. Graphene oxide (GO), prepared using the modified Hummers method, was used as the precursor matrix. Ethylene glycol was utilized as a solvent, dispersing medium, and mild reducing agent, while urea provided the nitrogen source. Sodium acetate was found to play a pivotal role in maintaining pH balance and facilitating iron oxide coprecipitation, while PEG-6000 functioned as a steric stabilizer. The formation of magnetite was accomplished through the utilization of $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$, in conjunction with microwave heating at an elevated temperature of 180°C for a duration of 30 minutes. The resulting material exhibited a homogeneous black coloration and a pronounced magnetic response, indicating a successful functionalization process. Scanning electron microscopy revealed the presence of spherical nanoparticles distributed over graphene oxide (GO) sheets, with diameters ranging from 20 to 50 nanometers. X-ray diffraction was used to confirm the disappearance of the characteristic GO peak and the emergence of reflections assigned to the spinel phase of magnetite. The FT-IR spectra indicated a partial reduction of GO, Fe–O vibrations, and nitrogen-containing groups, thereby supporting both magnetic functionalization and heteroatomic doping. Raman spectroscopy revealed a progressive increase in the I(D)/I(G) ratio, suggesting an escalating degree of structural disorder following successive modifications. Zeta potential values at pH 6.8 indicated moderate colloidal stability and a positively charged surface. In summary, the implementation of this one-step approach resulted in the successful development of a hybrid multifunctional material that exhibits considerable promise for utilization in diagnostic, imaging, and photoactivated applications.

We acknowledge financial support from FAPESP Grants 2024/10984-2 and 2024/02935-1, Brazil.

IM - D3 – P13

Dual crosslinked printable chitosan/PEG/γ-cyclodextrin hydrogels with tunable rheological properties

Semih Macit[1], Emre Akar[2], Hakan Durmaz[2], Yasemin Yuksel Durmaz[1,3]

[1]School of Engineering and Natural Sciences, Istanbul Medipol University, Türkiye; [2]Dept. of Chemistry, Istanbul Technical University, Türkiye; [3]Research Institute of Health Science and Technologies (SABITA), Istanbul Medipol University, Türkiye

3D bioprinting is an innovative technology that enables the layered production of living tissues, organs, and biomimetic structures. This technology is inspired by traditional 3D printing technologies but unlike them, it uses a special ink that allows cell adhesion. It is critical that these bioinks possess suitable rheological and mechanical properties that ensure fluidity during printing and maintain structural integrity after printing. In this study, printable hydrogel systems containing chitosan (Ch), poly(ethylene glycol) derivatives, and γ-cyclodextrin (γCD) with different crosslinking mechanisms were developed. The hydrogel systems were prepared using covalent crosslinking approaches based on amino-yne "click" reactions with PEG-DA and divinyl sulfone (DVS) as crosslinker, and combinations of these two systems were also investigated.[1] In addition to primary covalent bonds, hydrogen bonds formed through the hydroxyl groups of γCD provided secondary physical interactions, contributing to the structural integrity of the system. Thanks to this double crosslinking approach, flow was achieved by breaking physical bonds during printing, while covalent bonds and recovered hydrogen bonds maintained the stability of the structure after printing. Rheological analyses showed that the developed hydrogel systems exhibited a self-supporting structure with storage modulus in the range of 10^3–10^4 Pa and tanδ<1 values as shown in **Table 1**. Furthermore, it was determined that the systems exhibited shear thinning and thixotropic behavior. SEM analyses revealed that the hydrogels have a porous and interconnected internal structure. The findings indicate that the developed hydrogel systems are promising candidates for tissue engineering and biomedical applications.

Table 1. Rheological results of hydrogels.

Gel	η (Pa.s)	Max G' (Pa)	tanδ	Gelation T (℃)	90% Recovery (s)
CPGT1	516.8	3165.6	0.2	27.4	10
CPGT2	792.8	4812.9	0.3	28.5	25
CPGT3	1600	9790.4	0.2	20.0	5
CPdGD3	731.7	4533.9	0.2	32.7	9
CPdGD4	1349.2	8208.1	0.3	27.4	38
CPdGD5	250.4	1553.3	0.2	27.4	10

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IM - D3 – P14
Electrosynthesis of molecular cluster assembly materials with hierarchical porosity

Lara-Pauline Faden[1], Tom Althaus[2], Karen C. Bustillo[3], Natsuko Asano[4], Shunsuke Asahina[4], Shannon W. Boettcher[1,5], Alexander Katz[1]
[1]Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley, USA; [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), Germany; [3]National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA; [4]SMBU, JEOL, Akishima, Tokyo, Japan; [5]Dept. of Chemistry, University of California, Berkeley, USA

We report an electrochemically mediated assembly strategy that couples N-heterocyclic carbene (NHC)–protected tetrairidium clusters into one-dimensional oligomeric chains via direct metal–metal bonds, yielding self-assembled extended architectures with lengths of several nanometres. The hallmark is synthesis of these architectures with the molecular integrity of the individual clusters preserved. We demonstrate this approach across different cluster platforms starting with calix[4]arene-phosphine-protected triruthenium clusters, which are selected for their known propensity toward ring-opening reactions.[1] This concept is generalized with the attachment of a calix[4]arene-functionalized NHC ligand to a tetrairidium core[2,3] produces a hierarchically porous material. We demonstrate that the resulting molecular cluster assembled materials (MCAMs) exhibit emergent macroscopic properties that are highly dependent on the nature of the organic ligand, featuring interconnected pores with dimensions of several hundred nanometres and ultrathin walls down to 5 nm. Notably, the walls themselves are nanoporous, leading to a multiscale porous architecture that bridges molecular, nano-, and mesoscale organization. This approach provides a versatile bottom-up route to hybrid organic–metal materials from discrete molecular clusters, opening new opportunities for designing functional porous materials with tuneable structural and chemical properties relevant to catalysis and other functions relying on high exposed surface areas.

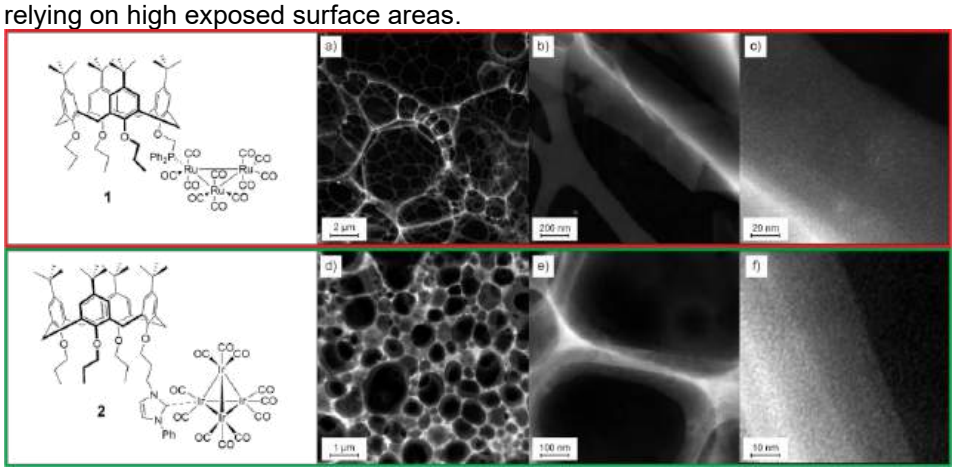

Fig. 1. Starting triruthenium cluster phosphine-complex 1 and starting tetrairidium cluster NHC-complex 2 with HAADF-STEM images with different magnifications of the MCAMs consisting of 1-red (a-b), and 2-red (d-f).

The authors acknowledge financial support from the DAAD through a PROMOS grant. This work was supported by the U.S. Dept. of Energy, Office of Basic Energy Sciences, under Grant No. DE-FG02-05ER15696. Electron microscopy was carried out at the National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, supported by the U.S. Dept. of Energy under Contract No. DE-AC02-05CH11231. The authors thank Zhongrui Zhou for ESI-MS measurements and Nick D'Antona for providing Pt/Ti-coated glass substrates.

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IM - D3 – P15
Twist and resist: Stability and chiroptical enhancement in chiral hybrid perovskites

Aleksandra Ciesielska[1], Wouter Van Gompel[1]
[1]Hasselt University, Institute for Materials Research (imo-imomec), Hybrid Materials Design (HyMaD), Belgium

Novel materials that are able to discriminate between left- and right circularly polarized light are in high demand for application in fields such as chiral optoelectronic technology and spintronics. With their unique blend of organic and inorganic components, 2D chiral hybrid perovskites (CHPs) have received increased interest due to their potential to be incorporated as active layer in CPL-LEDs, spin-LEDs and highly sensitive CD detectors. So far, the organic cations are equipped with an asymmetrical carbon atom to induce asymmetrical distortions to the inorganic framework (Fig .1), forming a semiconductor that is sensitive to the polarization of light. The hybrid character of this chiral semiconductor family offers a large degree of freedom regarding bandgap and energy alignment tuning. Nevertheless, CHPs are accompanied by a lower environmental stability than their achiral counterparts due to induced structural distortions by the chiral cations. This work focuses on increasing the intrinsic stability of 2D CHPs while maintaining chiroptoelectronic properties through tailored organic cation design.

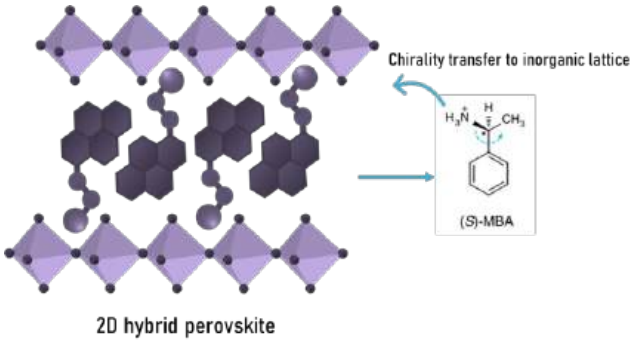

Fig.1. Representation of a 2D CHP

This research was funded by Fonds Wetenschappelijk Onderzoek (FWO) (research grant SB 1SH0X24N)

IM - D4 - P01

Enhancing the flame retardant performance of expandable polystyrene using halogen-free additives and synergists

Pinar Ozmen[1,2], Hayal Bulbul Sonmez[2]
[1]CFN Kimya Inc., Turkiye; [2]Gebze Technical University, Turkiye

The primary objective of this study is to synthesize and characterize expandable polystyrene (EPS) containing halogen-free flame retardant additives, and to evaluate its flame retardancy performance together with other critical properties, including mechanical strength, thermal stability, particle size distribution, and homogeneity. To accomplish this objective in a systematic and controlled manner, various halogen-free flame retardants with different functional groups are incorporated into the EPS synthesis process. This project aims to analyze the effects of flame retardants on flammability resistance, as well as monitoring their influence on the overall performance of the final EPS product. Special attention is given to ensuring that improvements in flame retardancy do not compromise the essential properties of EPS. Through systematic formulation development and optimization, the present research seeks to create a balanced material that exhibits enhanced fire resistance alongside optimized physical, mechanical, and thermal characteristics. This research contributes to the advancement of flame-retardant materials by providing a comprehensive understanding of how halogen-free flame retardants affect the synthesis and performance of EPS, thereby supporting safer and more sustainable applications across various industries.

IM - D4 - P02

Two salt-surfactant mesophases: Synthesis of mesoporous MgM_2O_4 (M=Mn, Fe and Co) electrodes and their electrochemical properties

Muratcan Ös[1], Ömer Dağ[1]
[1]Bilkent University, Turkiye

Mesoporous magnesium metal oxides or MgM_2O_4 (M=Mn (II), Fe (III) and Co (II)) have been synthesized by using transition metal nitrate salts including ([Mn $(H_2O)_4(NO_3)_2$], Co $(H_2O)_6(NO_3)_2$, and [Fe $(H_2O)_9(NO_3)_3$]), two surfactants; hexadecyltrimethylammonium bromide (CTAB), oligo (ethylene oxide) in water and ethanol as a solvent. This method of synthesis is called the molten salt-assisted self-assembly method (MASA), and The resulted clear solutions of the two salt-surfactant systems are lyotropic liquid crystalline phase (LLC) or mesophase features. The liquid crystal solutions and mesophases are analyzed using ATR-FTIR, XRD, and POM instruments. ATR-FTIR spectra for both salt surfactant samples show distinct features at 3600-3000 and 1650-1600cm^{-1}, which are related to stretching and bending modes of water species, respectively, as well as 1500-1290cm^{-1} due belongs to nitrate species. Low-angle XRD patterns show the ordered structure of LLC mesophases. The solutions are drop-cast coated over a glass substrate, calcined at elevated temperatures, and analyzed through high-angle XRD patterns. The crystallization starts even at 300 °C, and by calcination up to 700 °C, the corresponding mesoporous magnesium metal oxides are obtained. The porosity of the magnesium metal oxides is analyzed through XPS, and SEM.

Further, to investigate the catalytic performance of the samples in water oxidation, they are coated onto fluorine-doped tin oxide (FTO) substrates and subsequently calcined to obtain porous electrodes. These electrodes are then studied for their electrochemical properties using cyclic voltammetry (CV), and multi-step chronopotentiometry and amperometry (MCP-MCA) measurements. The results indicate that cobalt-based mesoporous electrodes have higher stability compared to manganese and iron-based electrodes, and exhibit small Tafel slope values in the range of 39–46 mV dec^{-1}, indicative of favorable reaction kinetics for water oxidation. The stability and electrochemical performance of those magnesium metal oxides are going to be tested over a graphite (GR) substrate.

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IM - D4 - P03

Calcone–schiff base hybride coated titanium surfaces with light-induced antibacterial activity

Çağla Akkol[1], Nurhayat Özbek[1], Fatma Demir[1], Salih Durdu[2,3], Ömer Kesmez[4], Nuran Kahriman[1], Ece Tuğba Saka[1], Miraç Ocak[1]

[1]Karadeniz Technical University, Türkiye; [2]Giresun University, Türkiye; [3]Giresun University, Türkiye; [4]Akdeniz University, Türkiye

Chalcone-based compounds incorporating a Schiff base hybride have attracted considerable interest due to their extended π-conjugation and versatile structural framework. Combining the chalcone (α,β-unsaturated carbonyl) and imine (–C=N–) functionalities enhances electronic delocalisation, resulting in enhanced optical, thermal and mesomorphic properties. These hybrid systems have been widely investigated for potential applications in nonlinear optics and liquid crystalline materials, as well as in bioactive agents with antibacterial, anticancer and antioxidant properties [1].

In this study newly synthesized chalcone schiff base hybride compound was coated onto titanium surfaces using the drop-casting method with a dimethylformamide (DMF) solution [2]. Following coating, XRD, SEM, EDX, FTIR and contact angle measurement tests were performed. The phthalocyanine-coated surfaces exhibited greater hydrophobicity than the uncoated surfaces. Activity tests against E. coli and S. aureus bacteria were then performed on the coated surfaces under both dark and daylight conditions.

Keywords: Chalcone, Schıff base, Titanium, antibacterial surface.

This work was supported by Karadeniz Technical University, Trabzon (Project Number:16509).

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IM - D4 - P04

Impact of PZA Incorporation on the thermal stability, carbon yield, and electrical conductivity of 3D-printed polymer-derived carbons

Noelia Corrochano Guijarro[1,2], Álvaro Grasa Alcázar[1], Jose L. Diaz de Tuesta[1,2*]
[1]Chemical and Environmental Engineering Group, Rey Juan Carlos University, Spain; [2]Instituto de Investigación de Tecnologías para la Sostenibilidad, Rey Juan Carlos University, Spain

This work investigates the thermal stability, carbonization behavior, and electrical performance of photopolymer-derived carbons obtained from resins containing different proportions of pyrazinamide (PZA) as a partial substitute for divinylbenzene (DVB). Among the PZA–DVB series, particular attention was given to samples MDVB (0% PZA) and MPZA (100% PZA), which represent the two compositional extremes and therefore enable elucidation of the structural effects induced by PZA incorporation on the properties of the resulting pyrolytic carbon. Both materials were fabricated via vat photopolymerization followed by thermal pre-oxidation at 300°C and pyrolysis at 900°C under nitrogen, following similar methods than those previously published [1-2]. Mass yield measurements revealed a strong dependence on PZA content: while MDVB retained 20.0% of its mass after pyrolysis, MPZA exhibited a markedly lower final yield of 5.7%, indicating extensive volatilization and structural fragmentation in the PZA-rich resin. Consistent with this trend, MPZA also displayed significantly higher volume shrinkage (~94%) compared to MDVB (~84%) (Figure 1.a-b), confirming that PZA alters the degradation pathway and reduces the char stability of the polymer network. Thermogravimetric analysis (TGA) further showed that the precursor MDVB oxidize at higher temperatures than MPZA (Figure 1.c), while both pyrolyzed materials exhibit the characteristic high thermal stability of carbonaceous solids under nitrogen atmosphere. Proximate and elemental analyses confirmed the substantial increase in fixed carbon content after pyrolysis (MDVB: 93.8%; MPZA: 82.9%), along with a drastic reduction in H/C ratios, indicative of extensive aromatization. Nitrogen incorporation was higher in the PZA-rich sample (Figure 1.d), validating PZA as an efficient nitrogen source. Electrical conductivity measurements revealed that MPZA achieves significantly higher conductivity (~1037 S/m) than MDVB (~155 S/m). These results demonstrate that PZA strongly influences carbon yield, nitrogen incorporation, microstructural evolution, and electrical performance in polymer-derived 3D carbon architectures.

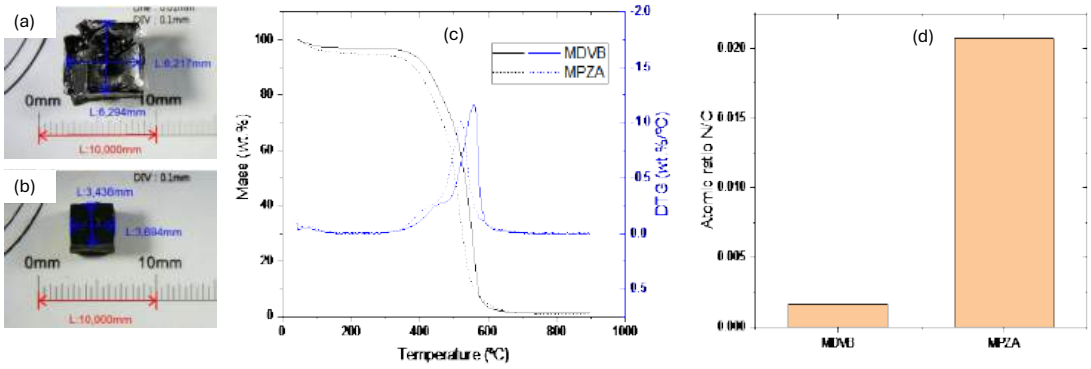

Fig. 1. Photographs of (a) sample MDVB and (b) sample MPZA, (c) TGA and (d) atomic ratios N/C obtained by elemental analysis.

Acknowledgements: The authors would like to express their sincere gratitude to the DACIU Program (*Desarrollo de las Altas Capacidades Intelectuales en la Universidad*) of Fundación Avanza for its support. Noelia Corrochano Guijarro and Jose L. Diaz De Tuesta acknowledge financial support through the grant 2022-T1/AMB-23946 funded by *Comunidad de Madrid*. Jose L. Diaz De Tuesta also acknowledges the financial support through the grant CNS2024-154264 funded by *Agencia Estatal de Investigación*.

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IM - D4 - P05
3D printing of nanocomposites-some assembly required

Aoife Donohue[1], Aoife M. Morris[1], Teodora Faraone[1], Colm Delaney[1]
[1]School of Chemistry & AMBER, the SFI Research Centre for Advanced Materials and BioEngineering Research, Trinity College Dublin, Ireland

Using just a handful of raw material building blocks, nature has succeeded in using different design and fabrication strategies to yield a broad canvas of hierarchical structures. To date, the generation of synthetic photonic materials has followed two diverse routes which have made considerable progress in separately delivering intrinsically and extrinsically ordered materials. Intrinsically photonic materials have been achieved through self-assembly protocols, such as evaporation-induced self-assembly, shear alignment, and application of magnetic field. Attention in this field has also been garnered by renewable biopolymers such as guanine, cellulose nanocrystals, hydroxypropyl cellulose.[1-4] Extrinsic structuring for the generation of photonic devices has focussed on techniques borrowed from micro-electro-mechanical systems (MEMS) technologies, such as e-beam lithography and wet chemical etching in silicon, glass, metals, diamond, and other high refractive-index dielectrics.
Creating responsive optical elements with multiple components requires a holistic approach which marries smart material development with cutting edge fabrication techniques to combine intrinsic and extrinsic structuring.[5,6]
Herein, this is realised through the combination of three elements: 1) two-photon polymerisation (2PP) for the generation of biomimetic structures with extrinsic order; 2) nanomaterial dispersions to alter the refractive index of hydrogels and achieve a photonic bandgap within the polymeric matrix and; 3) stimuli-responsive hydrogels that exhibit a controllable response under stimulation.

Fig. 1. Schematic of direct laser writing process in ordered photoresists. a) Polymerisation being achieved in a voxel-by-voxel manner. b) The effect of fabrication parameters on the assembled nanocomposite. c) Response of photonic arrays in response to chemical stimuli.

C.D. acknowledges funding from Research Ireland under the Pathway Programme (Grant No. 22/PATH-S/10790).

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IM - D4 - P06
Silica-based degradable micromotors with potential environmental and health impact

Yolanda Salinas, Amelie Krug, Uwe Rinner
IMC Krems University of Applied Sciences, Institute of Applied Chemistry, Austria

Degradable nanomaterials are increasingly recognized as a key enabler in tackling global sustainability challenges. Future material design must not only ensure safety and reduced ecological footprint, but also maintain, or ideally enhance, functional performance. Our research focuses on silica-based nanomaterials engineered with programmed degradability. Introducing controlled breakdown mechanisms significantly broadens their application scope, ranging from drug delivery systems and biomedical release platforms[1] to analytical technologies and environmental remediation strategies. To achieve this, we have integrated emerging degradable components, such as polyphosphazene segments, directly into the silica network. This approach has led to the development of advanced hybrid porous nanostructures that might combine on-demand functionality response with controlled tunable degradability (Figure 1).[2-5] Beyond static applications, we have extended these concepts to dynamic systems by designing silica-based micro/nanomotors. We demonstrated precise activation, deactivation, and directional control through a reversible external braking mechanism based on thermoresponsive bottle-brush polymers.[6-7] Despite these promising results, such complex motorized architectures require further investigation, particularly regarding navigation accuracy and controlled propulsion in biologically relevant microfluidic environments.

The Institute of Applied Chemistry acknowledges the funding for the project “Micromotors and nanomaterials for ecological applications” (DEGMOT) WST3 - F-5030820/028-2024

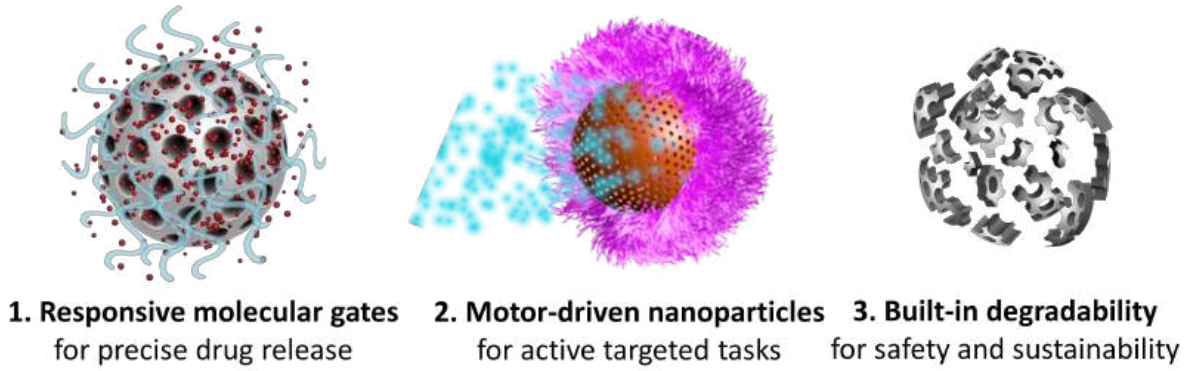

Fig. 1. Innovative micromaterials that safely break down after use, standing on three pillars

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IM - D4 - P07

Efficient dissolution and selective recovery of gold from electronic waste using a recyclable ionic medium

Abhijit Nag[1]*, Abinash Swain[2], Mudila Dhanunjaya Rao[3], Jacob Lynge Elholm[1], Vitor A. S. Almodovar[1], Rohit B Meshram[3], Pankaj Bharmoria[1], Helen Hölzel[1,4], Kamalesh K Singh[5], Guillem Aromí[2], Kasper Moth-Poulsen[1]*
[1]Universitat Politècnica de Catalunya, Spain; [2]Universitat de Barcelona, Spain; [3]CSIR- National Metallurgical Laboratory, India; [4]Justus-Liebig-Universität Giessen, Germany; [5]Indian Institute of Technology (Banaras Hindu University), India
**Corresponding author*

The significant socio-economic and technological importance of gold necessitates sustainable supply to meet the continuously rising demand. As the demand rises, recovering gold from secondary sources has become increasingly important, highlighting the need for environmentally and economically sustainable extraction processes.[1-5] In this study, gold was efficiently and rapidly leached quantitatively as Au(III) halometalate (Cl/Br) complexes and selectively recovered (~100%) in eight different hydrophobic ionic liquids (ILs) based on pyridinium, pyrrolidinium, and imidazolium at room temperature from both mixed metals solution and electronic waste (e-waste). ILs were recovered after extraction, and used for another two cycles for dissolution and recovery of gold thus demonstrating the economic sustainability of the developed process. Moreover, a techno-economic analysis of the method reveals attractive numbers for gold recovery, even without recycling of ILs. The background for the selective chemistry was studied comprehensively using diverse analytical techniques, complemented by density functional theory (DFT) calculations, and life cycle analysis (LCA). Furthermore, single crystal X-ray diffraction and DFT calculations revealed that non-covalent interactions between the cationic part of the IL and Au(III) halide are key for selective gold separation. The LCA study demonstrates that the process can lower CO_2 emissions by ~84.4% compared to conventional gold mining under the current Indian energy mix, with the potential for an almost complete emissions reduction (~99.9%) if powered by solar energy. The developed process is expected to pave the way for economic and environmentally sustainable recycling of multi-metals from e-waste.

Acknowledgements: A.N. and K.M.P. acknowledges the Marie Skłodowska-Curie Actions–European Commission post-doctoral grant (REWCHEM, Grant agreement ID: 101152892) and Sustain-a-Print project (Grant agreement ID: 101070556) from European Commission for research funding. P. B. acknowledges, Ramón y Cajal grant from Spanish State Investigation Agency (Grant no. J03416).

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IM - D4 - P08
Magnetically induced drug release from doxorubicin-loaded niosome nanocarriers

Philip Drake[1*], Ilma Amalina[2], Retno Sari[3], Amalia Ruiz[4], Saliha Ramazan[1], Gordon Hope[1], Dharmisthaben Pancholi[1], Andang Miatmoko[3]
[1]School of Chemistry and Biosciences, Faculty of Life Sciences, University of Bradford, UK; [2]Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Saudi Arabia; [3]Dept. of Pharmaceutical Sciences, Faculty of Pharmacy, Universitas Airlangga, Indonesia; [4]Institute of Cancer Therapeutics, University of Bradford, UK

Niosomes is vesicular nanocarriers composed of nonionic surfactants and cholesterol which have emerged as versatile systems for controlled drug delivery due to their high biocompatibility, structural stability, and ability to encapsulate both hydrophilic and hydrophobic drugs.1,2 This study aims to design and evaluate a magnetically stimuli-responsive niosomal system for the control release of the anticancer drug doxorubicin under alternating magnetic field exposure. The formulation combined doxorubicin and magnetic nanoparticles loaded niosomes for controlled release cancer therapy. Dextran coated iron oxide magnetic nanoparticles were synthesized by a co-precipitation method under a nitrogen atmosphere3,4 and niosomes were synthesized by the thin-film hydration technique made of Span 60 and cholesterol.5 The loading efficiency of the doxorubicin was between 60–70%. The hydrodynamic diameter measured as the average number was found to be 188 ± 68, 141 ± 86 and 169 ± 69 nm for the plain niosomes, niosomes-doxorubicin and niosomes-doxorubicin-magnetic nanoparticles, respectively. The thermally mediated release of doxorubicin was monitored using fluorescence spectroscopy and found to follow 1st order kinetics. The doxorubicin was also released using an alternating magnetic field, this also followed 1st order kinetics with a rate constant of 1.7x10-2 min-1. This is four orders of magnitude greater than the thermal release at the same temperature (298 K). The work shows the magnetically controlled, burst release from a drug-loaded niosome delivery system. The release was triggered on demand by the application of the alternating magnetic field, resulting in 86% doxorubicin release within 3 hours.

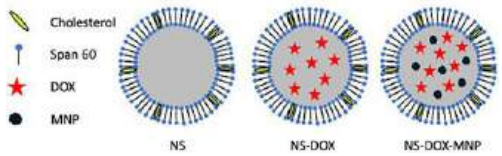

Fig. 1. An illustration of the niosome samples prepared. NS, DOX and MNP stand for niosome, doxorubicin and magnetic nanoparticles respectively.

Acknowledgements: This research was supported by the Royal Society of Chemistry (E22-5590558249), the University of Bradford and Airlangga University and the University of Leeds for electron microscopy and spectroscopy analysis and KFUPM for conference grant.

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IM - D4 - P09
Exploring composite hydrogel systems using solid state NMR

Roderick Abdilla[1], Ruben Gatt[1], Sander Lambregts[2], Nicola Agius[1]
[1]Metamaterials unit, Chemistry Dept., University of Malta, Malta; [2]IMM Magnetic Resonance Research Centre, Radboud University, The Netherlands

Hydrogels are structurally complex, heterogeneous polymer networks whose functional properties depend strongly on molecular-level interactions that remain challenging to characterise. In this work, solid-state nuclear magnetic resonance (ss NMR) spectroscopy is employed to investigate the structure and intermolecular interactions within a range of composite hydrogel systems based on poly(vinyl alcohol) (PVA).
Five hydrogel formulations were examined, including PVA–gelatin–chitosan composites, glutaraldehyde-crosslinked PVA with sodium alginate, PVA–TEOS hybrid networks with oxidized alginate, β-cyclodextrin-incorporated systems (Figure 1), and silica-supported flavylium dye-functionalised materials. ^{13}C CP/MAS NMR provided detailed insight into polymer backbone structure, crosslinking behaviour, and chemical environments, while ^{1}H ss NMR revealed changes in molecular mobility and hydrogen-bonding interactions.
Results indicate that, in the PVA–gelatin–chitosan system, interactions are predominantly non-covalent, with limited esterification under aqueous conditions. In contrast, glutaraldehyde and TEOS-based systems exhibit clear evidence of covalent crosslinking through acetal and siloxane linkages, respectively. Incorporation of oxidized alginate introduces additional hemiacetal/acetal structures, leading to increased network heterogeneity and reduced chain mobility. The inclusion of β-cyclodextrin and functional additives further modifies the hydrogen-bonding network and structural organisation, while immobilisation of flavylium dyes on silica demonstrates altered molecular environments and restricted mobility.
Overall, this study highlights the capability of ss NMR to resolve complex structural features in hydrogel systems, providing critical insight into the relationship between composition, intermolecular interactions, and material properties.

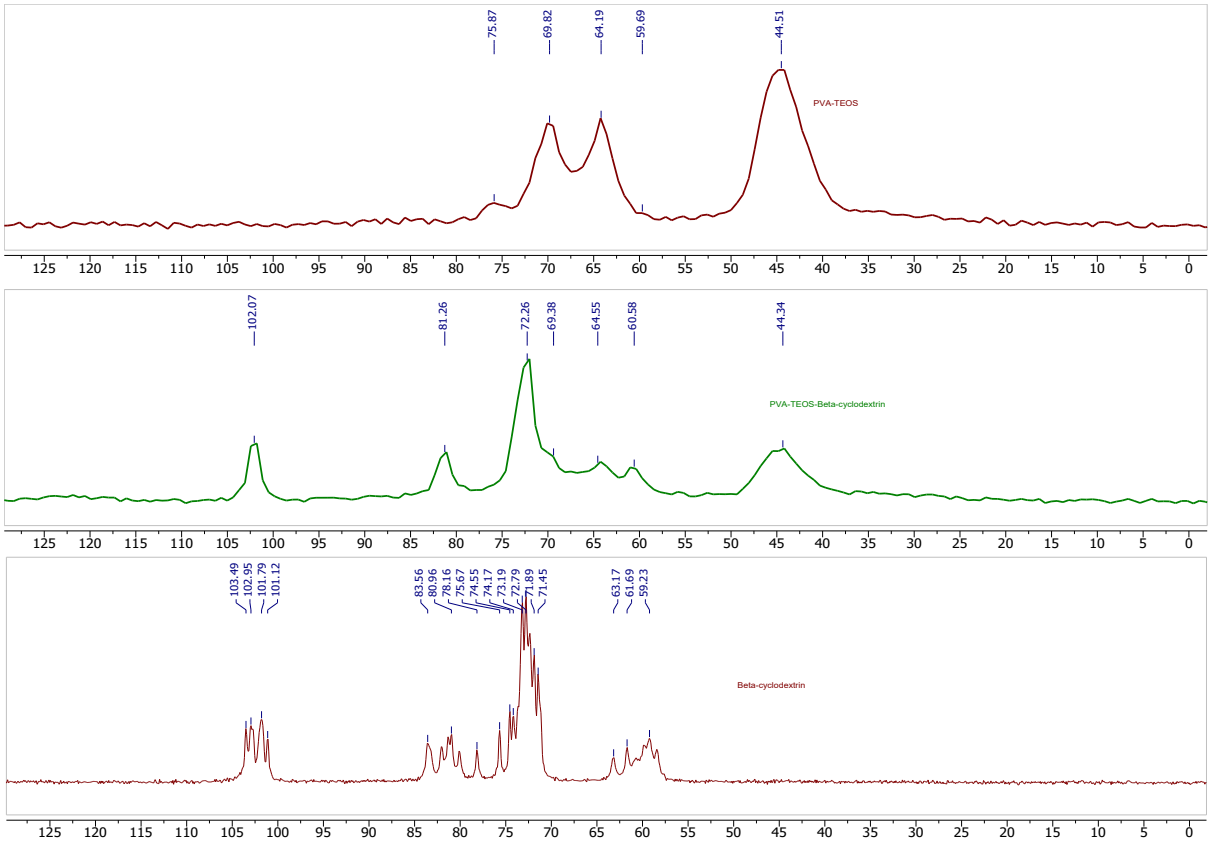

Fig.2. Stacked ss CP/MAS ^{13}C NMR spectra of PVA-TEOS film, PVA-TEOS film incorporated with cyclodextrin and of β-cyclodextrin

The authors acknowledge financial support from the European Union under the Horizon 2020 program Panacea within a contract for Integrating Activities for Starting Communities, contract number 101008500. They also acknowledge the infrastructure and assistance given at the University of Malta.

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IM - D4 - P10

A multifunctional nitrogen-doped magnetic graphene oxide nanocomposite prepared by one-step microwave-assisted synthesis

Émerson Leandro-Silva[1], Luiz Carlos Silva-Filho[1], Marina Piacenti-Silva[1]
[1]School of Sciences, Unesp, Brazil

This work reports the synthesis and characterization of a multifunctional nanocomposite based on magnetite-functionalized graphene oxide (mNGO), obtained through a one-step microwave-assisted hydrothermal route. The proposed strategy was designed to provide a rapid and controllable method for producing hybrid materials with integrated magnetic and photoactive properties. Graphene oxide (GO), prepared using the modified Hummers method, was used as the precursor matrix. Ethylene glycol was utilized as a solvent, dispersing medium, and mild reducing agent, while urea provided the nitrogen source. Sodium acetate was found to play a pivotal role in maintaining pH balance and facilitating iron oxide coprecipitation, while PEG-6000 functioned as a steric stabilizer. The formation of magnetite was accomplished through the utilization of $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$, in conjunction with microwave heating at an elevated temperature of 180°C for a duration of 30 minutes. The resulting material exhibited a homogeneous black coloration and a pronounced magnetic response, indicating a successful functionalization process. Scanning electron microscopy revealed the presence of spherical nanoparticles distributed over graphene oxide (GO) sheets, with diameters ranging from 20 to 50 nanometers. X-ray diffraction was used to confirm the disappearance of the characteristic GO peak and the emergence of reflections assigned to the spinel phase of magnetite. The FT-IR spectra indicated a partial reduction of GO, Fe–O vibrations, and nitrogen-containing groups, thereby supporting both magnetic functionalization and heteroatomic doping. Raman spectroscopy revealed a progressive increase in the I(D)/I(G) ratio, suggesting an escalating degree of structural disorder following successive modifications. Zeta potential values at pH 6.8 indicated moderate colloidal stability and a positively charged surface. In summary, the implementation of this one-step approach resulted in the successful development of a hybrid multifunctional material that exhibits considerable promise for utilization in diagnostic, imaging, and photoactivated applications.

We acknowledge financial support from FAPESP Grants 2024/10984-2 and 2024/02935-1, Brazil.

IM - D4 - P11

Multifunctional novel materials for CO_2 capture and nutrient delivery: Advanced soil amendments to enhance soil health and crops growth

Faizah Altaf[1], Safyan Akram Khan[1*]

[1]Interdisciplinary Research Center for Hydrogen and Energy Storage (IRC-HES), King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia

This study presents the synthesis and evaluation of multifunctional materials (MFs) designed for simultaneous CO_2 capture and soil fertility enhancement, addressing challenges of desertification, carbon emissions, and poor soil productivity in arid regions. Composite formulations were prepared using sand, montmorillonite clay, humic acid, and charcoal, individually and in combination, with polyethyleneimine (PEI) surface modification to introduce amine-rich functional groups for improved chemisorption and nutrient interaction. Characterization through FTIR, XRD, SEM, and BET confirmed successful functionalization, enhanced surface area, and stable structural morphology. The materials displayed varying CO_2 adsorption capacities (0.025–4.5 mmol/g), with MF-12 achieving the highest performance due to synergistic interactions among PEI, clay, humic acid, and carbon phases. Water retention increased from 5% in pure sand to 38% in the best-performing composite. Electrical conductivity (0.406–0.537 mS/cm) remained within the optimal range for nutrient availability. In coriander growth trials, MF-12 demonstrated superior plant height, biomass, and petal development, confirming improved water retention and nutrient cycling. The study establishes that PEI-modified organic–inorganic composites are highly effective as multifunctional soil amendments capable of capturing atmospheric CO_2 while enhancing soil moisture, conductivity, and plant productivity, offering a sustainable solution for climate-resilient agriculture.

IM - D4 - P22

Systematic functionalization of silk sericin via acetylation: A design of experiments approach toward sustainable biomaterials

Rony Aad[1], Luca Leuzzi[2], Diletta Ami[2], Greta Bianchi[2], Marco Mangiagalli[2], Antonino Natalello[2], Laura Cipolla[2], Simone Vesentini[1]

[1]Politecnico di Milano, Italy; [2]University of Milano-Bicocca, Italy

Silk sericin, the glue-like protein that binds fibroin fibers within silk, is generated in large quantities as an industrial byproduct and discarded despite its rich chemical functionality. Its intrinsic properties, including biocompatibility, biodegradability, antioxidant activity, and antibacterial behavior, make it a promising candidate for bio-based materials; however, its effective valorization remains limited by the lack of a quantitative understanding of the relationship between chemical modification and structural evolution. Here, a quantitative framework is established to investigate and control sericin functionalization using acetylation as a model reaction, which was selected for its ability to tune the degree of functionalization and secondary structure organization while introducing a biodegradable ester functionality. A Design of Experiments (DoE) approach was employed to systematically assess the effects of acetyl chloride equivalents, initial sericin concentration, and lithium chloride content, including their interaction effects. Fourier-transform infrared (FTIR) spectroscopy was advanced as a quantitative, model-integrated analytical approach. Band deconvolution across the Amide I region (1780–1580 cm^{-1}) enabled the extraction of two complementary descriptors, defined as the functionalization index (FI) and β-sheet index (BI), derived from band areas and intensities. The resulting models exhibited strong predictive capability and statistical significance ($p < 0.01$), with good agreement between experimental and predicted responses. Notably, the system displayed pronounced non-linear behavior governed by significant quadratic and interaction effects, revealing a multidimensional response surface. These findings demonstrate a direct coupling between chemical reactivity and protein structural organization, enabling predictive control over sericin modification. Overall, this work introduces a reproducible and quantitative methodology for linking reaction parameters to both chemical and structural outcomes, supporting the development of sericin as a sustainable, high-value biomaterial platform.

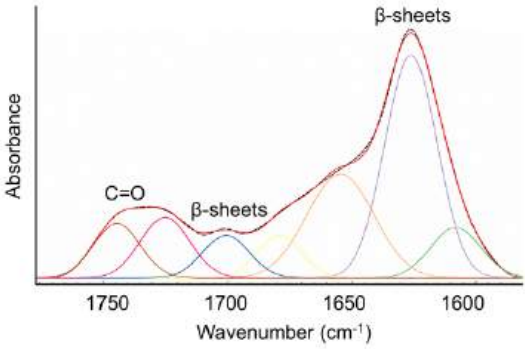

Fig.1. FTIR band deconvolution illustrating the extraction of functionalization and β-sheet structural descriptors.

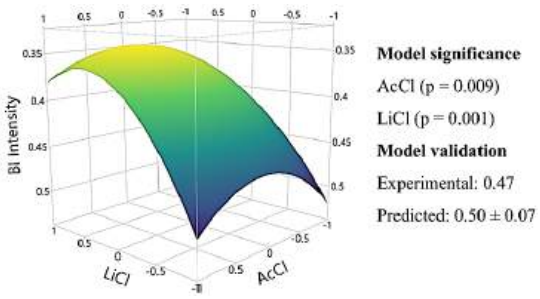

Fig. 2. Response surface of BI (intensity) highlighting the effects of AcCl and LiCl, with model significance and validation.

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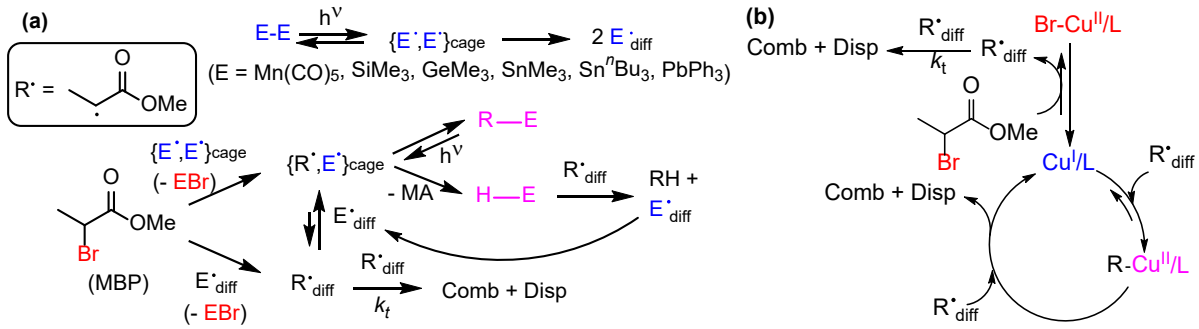
Posters

Molecular Design & Reactivity (MDR)

MDR - D1 - P01
How do acrylate radicals terminate? New evidence to settle a never-ending debate

Laurianne Forget[1], Krzysztof Matyjaszewski,[2] Christophe Fliedel,[1] Rinaldo Poli[1]
[1]Laboratoire de Chimie de Coordination (LCC CNRS), CNRS, Université de Toulouse, France; [2]Dept. of Chemistry, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA

Radicals are reactive species of interest in many areas, such as organic synthesis, biochemistry and polymer science, but they have a short life, spontaneously terminating in bimolecular processes by combination (Comb) and/or disproportionation (Disp). While the termination mode is well established for radicals such as primary alkyls, cyanoalkyls, styryl and methacrylates, the preferred termination mode of acrylate radicals is still under debate, some evidence pointing to the prevalence of Disp,[1] others to nearly 100% Comb.[2] The analysis is complicated by the unavailability of a suitable azo derivative, *e.g.* (MeOOC)CH(Me)N=NCH(Me)(COOMe). Thus, investigations have to rely on complex and indirect methods.
We have now investigated the termination of the carbomethylethyl radical, •CH(Me)(COOMe), generated by Br-atom abstraction from methyl 2-bromoproprionate (MBP) by either a stronger heteroatom radical, E•, obtained by photolysis of stable E-E precursors (E = $Mn(CO)_5$, $SiMe_3$, $GeMe_3$, $SnMe_3$, Sn^nBu_3, $PbPh_3$), or a copper(I) complex. The investigations show that other phenomena (such as radical trapping by E• and H-atom transfer, **a**, or catalyzed radical termination, **b**) interfere with the spontaneous bimolecular radical termination process, skewing the Disp/Comb ratio. A combination of experimental and DFT mechanistic studies, however, shed new light on this controversial issue.



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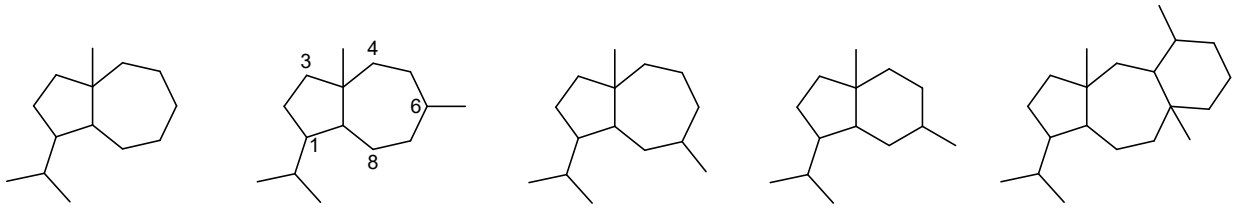
MDR - D1 - P02

Verification, falsification and revision of the constitution and configuration of daucane sesquiterpenoids based on total synthesis and X-ray crystallography

Josefine Brindöpke[1], Adrian Dennis Podlesny[1], Martin Hiersemann[1]
[1]Technische Universität Dortmund, Germany

Natural products based on the daucane (carotene) or isodaucane backbone have been isolated from plants, fungi, or marine life forms (Figure 1).[1] Based on the ex-chiral-pool access to a versatile five-membered building block, we envision a unified annulative approach to the nordaucane, daucane and isodaucane scaffolds. The daucane sesquiterpene backbone is also contained in the dolastane diterpene backbone. Accordingly, dolastanoids should be accessible from daucanoids by a second suitable annulation reaction. On our poster we report on our access to the daucane, nordaucane and isodaucane backbone and on the ex-chiral-pool total synthesis of corresponding natural products.

Fig. 1. Daucane, isodaucane, nordaucane and dolastane scaffolds.



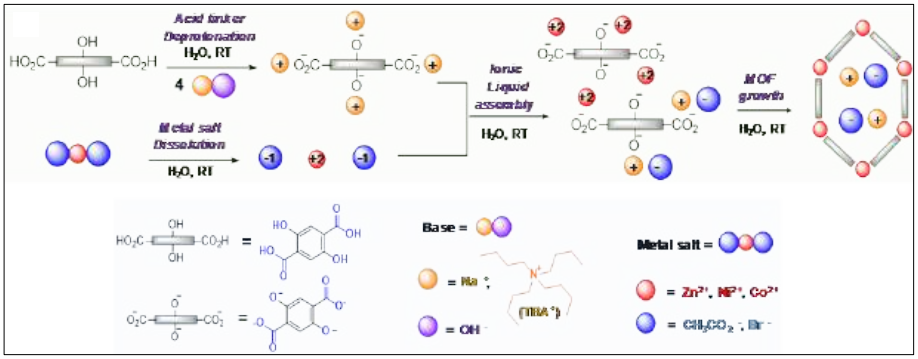
6-nordaucane daucane isodaucane nordaucane dolastane

[1]Ghisalberti, E. L. *Phytochemistry* **1994**, *37*, 597–623.
[2]Hiersemann, M.; Helmboldt, H. *Top. Curr. Chem.* **2005**, *243*, 73–136.

MDR - D1 - P03
Green ionic metal-organic frameworks as nanocatalysts for CO2 fixation

F. G. Cirujano[1*], N. Martín[1*], M. Maireles-Porcar[1], J. Sánchez Velandia[1], B. Altava[1] and E. García-Verdugo[1*]
[1]Universitat Jaume I, Castelló de la Plana, Spain

This study introduces a green, one-pot synthesis for incorporating ionic liquids (ILs) into metal-organic frameworks (MOFs) to enhance CO2 fixation. By using strong bases and metal bromides in water, the method eliminates toxic solvents and enables the simultaneous formation of MOFs (such as M2(dot) with metals like Zn, Co, and Ni) and ILs (Scheme 1).[1] This approach improves catalytic performance for CO_2-epoxide cycloaddition, producing bio-based plastics with a lower carbon footprint. It also reduces the need for co-catalysts and high pressure, offering a more sustainable solution for CO_2 fixation.
We developed a fast room temperature aqueous synthesis of Co, Ni, and Zn iso-reticular coordination polymers of 2,5-dihydroxyterphthalic acid using metal bromides and tetrabutylammonium hydroxide (TBAOH) as the base resulting in MOF-ionic liquid composite materials.
We show the key role of the base and metal salt employed in the MOF synthesis, allowing the formation of ionic liquids within the MOF structure in the case of using metal bromides and alkyl ammonium bases as deprotonating and directing agents of both linkers and final MOF nanocrystals. The structure and composition have been thoroughly characterized using techniques such as XRD, SEM, FTIR, TGA, XPS, and elemental analysis. These TBA@M_2dot ionic-liquid/MOF hybrid materials can promote the CO_2 cycloaddition to epoxide with one of the highest TONs reported so far, i.e. up to 700, exhibiting adequate ionic liquid-MOF interactions which allow for use as a heterogeneous catalyst during different reaction cycles with minor decrease in catalytic activity. The proposed materials allow employing at least ten times less TBABr (i.e. 0.3%wt.), and less than 1%wt. of metal (0.7-0.9%wt.) with respect to the epoxide at just 1 bar of CO_2 (balloon).



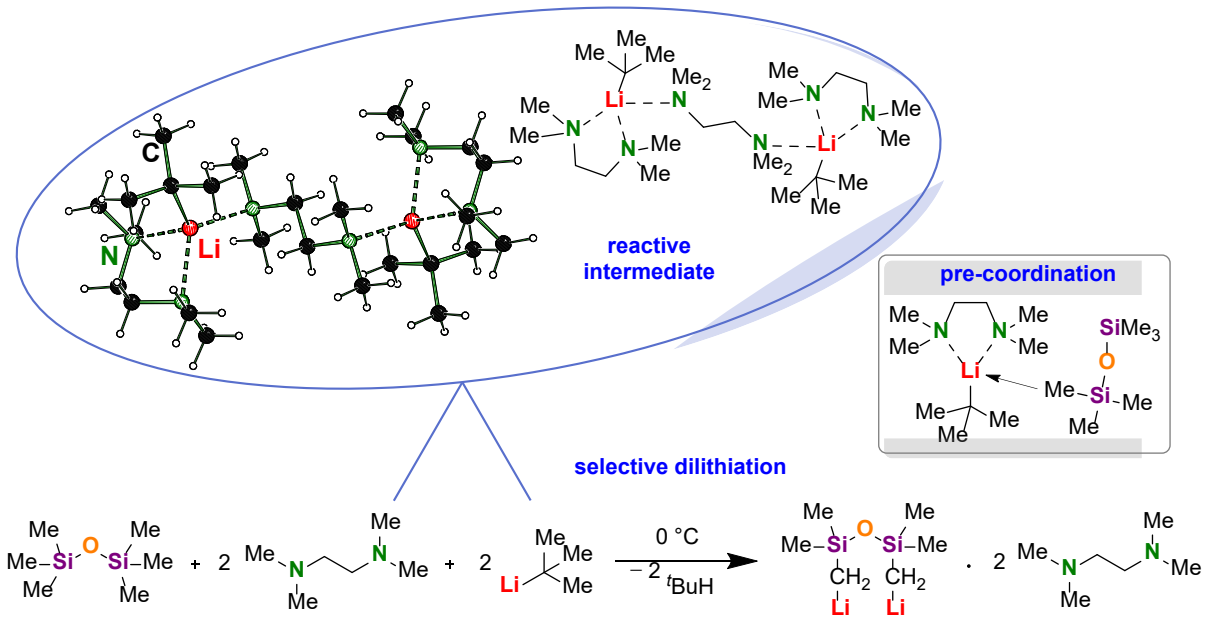
Scheme 1. Design of MOF-ILs as catalysts for CO_2 fixation into carbonates.

[1]Martín, N. et al. *NanoResearch* **2025**, *18,* 94907069.

MDR - D1 - P04
Why can we deprotonate methylsiloxanes with the combination of *t*-BuLi and TMEDA?

Mara Schöler[1], Johannes Kleinheider[1], Tristan Mairath[1], Rebecca Scheel[1], Carsten Strohmann[1]
[1]*Faculty of Chemistry and Chemical Biology, TU Dortmund University, Germany*

Alkyllithium reagents like *n*-BuLi can be activated by the diamine TMEDA due to the formation of small aggregates.[1,2] A more reactive reagent needed for deprotonations of unreactive substrates like methylsilanes was found to be the combination of *t*-BuLi and one equivalent of TMEDA.[1,2]
Normally, reactive reagents consisting of an alkyllithium compound and ligands require at least one free coordination site to enable deprotonations of weak pre-coordinating substrates.[2] Using THF as a ligand, the lithium center is triple coordinated by three THF molecules and thus, substoichiometric amounts of THF are needed to create a free coordination site.[2]
Herein, we combined two equivalents of each TMEDA and *t*-BuLi and obtained a coordination polymer. While the lithium center of *t*-BuLi is usually only coordinated by two nitrogen atoms, the obtained complex reveals a triple nitrogen coordinated lithium center.[1] The bidentate ligand TMEDA not only directly coordinates through its two nitrogen centers, but additionally acts as a bridge between two lithium centers. Therefore, one nitrogen atom coordinates comparably weaker than the others so that we obtain a latently free coordination site combined with a small alkyllithium aggregate. TMEDA shows a bifunctional behaviour in this coordination compound and the formed reagent should be highly reactive at low temperatures.
Usually, selective deprotonation reactions of methylsiloxanes are kinetically hindered due to the partial negative charge of the methyl groups.[2] By inducing a competition between the weakly coordinating third nitrogen center of TMEDA and a methyl substituent of the siloxane, selective mono- and even dilithiation can be achieved.



Scheme 1. Selective dilithiation of hexamethyldisiloxane via the reactive intermediate formed by TMEDA and *t*-BuLi.

[1]Gessner, V. H.; Däschlein, C.; Strohmann, C. *Chem. Eur. J.* **2009**, *15*, 3320–3334.
[2]Kleinheider, J.; Schrimpf, T.; Scheel, R.; Mairath, T.; Hermann, A.; Knepper, K.; Strohmann, C. *Chem. Eur. J.* **2024**, *30*, e202304226.

MDR - D1 - P05
Development of synthetic methods for terpyridine-based solid molecular catalysts

Felix Friedt[1], Regina Palkovits[1,2]
[1]Institute of Technical and Macromolecular Chemistry, RWTH Aachen, Germany; [2]Institute for a Sustainable Hydrogen Economy, Forschungszentrum Jülich GmbH, Germany

In the field of catalysis, the conventional divide between homogeneous and heterogeneous catalysis can be overcome by solid molecular catalysts (SMCs). These materials combine the stability of heterogeneous catalysts with molecularly defined active sites.[1] One possibility for achieving such materials is the incorporation of coordination sites into tailorable polymeric solids. This concept, derived from covalent organic frameworks, has been demonstrated to provide tunable and well-defined active sites in combination with materials whose bulk characteristics can be influenced by the strategic choice of monomer molecules.[2] These advantages are further elevated by their high degree of metal utilization, thus offering a more sustainable alternative.
In this work, we describe different approaches of a straightforward, low-cost, metal-free synthetic strategy for terpyridine-based SMCs. The strategic use of multivalent, heteroaromatic monomers leads to the perpetuation of a polymeric network in which the formation of the center pyridine ring of the terpyridine motive is the driving force. After the development of this polymerization, it was possible to adapt the procedure for an expanding monomer scope to influence catalytic performance and bulk characteristics of the materials. We were further able to adapt the reaction from a solvothermal to a microwave and mechanochemical synthesis, shortening reaction times drastically. The synthesized polymeric materials can then be utilized in different catalytic processes and tailored for the specific application. We were thus able to achieve significant results in both metal-free photocatalytic reactions as well as metal-mediated formic acid dehydrogenation through the coordination of iridium to the motive.

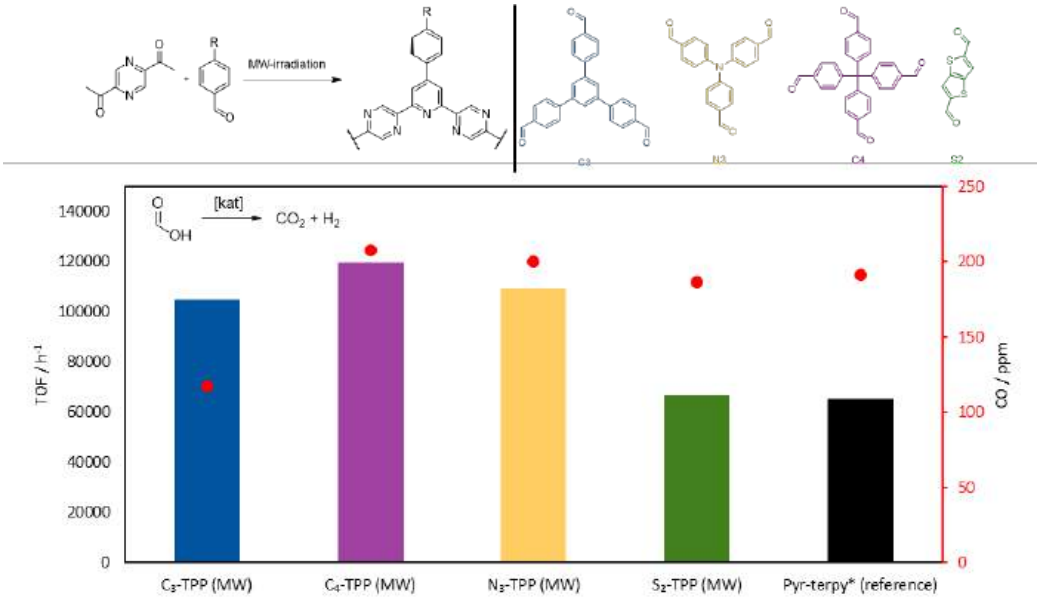


Fig. 1. Synthetic pathway and aldehyde scope of microwave terpyridine polymer (TPP) materials with formic acid dehydrogenation results, including TOF and CO content. Parameters: 15 mg catalyst (1 wt% Ir), 6 mL formic acid solution (10 wt%), 160 °C, 750 rpm, 1 h in Hastelloy steel autoclaves.

This work was funded by the Cluster of Excellence Fuel Science Center (EXC 2186, ID: 390919832) of the Excellence Initiative of the German federal and state governments.

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[2]Birkelbach, K. V. A.; Vossen, J. T.; Rösler, T.; Kappel, I.; Meise, A.; Heggen, M.; Vorholt, A. J.; Palkovits, R. Angew. Chem. Int. Ed. 2025, 64, e202424144

MDR - D1 - P06
Coordination chemistry of a ferrocenyl terpyridine-like ligand: Electrochemical sensing of metal ions

Márk Váradi[1], Mátyás J. Gazsi[1], Lajos Fodor[1], Rita Skoda-Földes[1]
[1]University of Pannonia, Center for Natural Sciences, Hungary

2,2';6',2"-Terpyridine type molecules are tridentate ligands that possess unique structure and exceptional coordination abilities. Their electronic and geometric adaptability renders them valuable building blocks in the design of sensory molecules, catalyst systems and photosensitive materials.[1] Taking advantage of the redox activity of ferrocene, electrochemical properties of some transition metal (Fe, Rh, Co) complexes of 4'-ferrocenyl-terpyridine ligands had been investigated in detail.[2]
In continuation of our previous work concerning the application of ferrocenylpyrimidine derivatives in the sensing of neutral molecules[3] or strong acids,[4] terpyridine analogue **L** (Figure 1) with ferrocenylpyirimidine moieties was synthesised starting from ferrocenecarboxaldehyde. Formation of ML_2- and ML-type complexes upon the addition of triflate or acetate salts of various metals (Cu^{2+}, Zn^{2+} and Fe^{2+}) was followed by UV-Vis and CV titrations, and eventually, by NMR spectroscopy.
Ratios of the different species and their stability- and association constants were calculated based on UV-Vis titrations. The formation of ZnL and ZnL_2 complexes could also be followed by NMR spectroscopy. Quantum chemical calculations were used to assist interpretation of NMR spectra. Electrochemical measurements showed that anodic peak potentials of the complexes depended on the nature of the metal ions. Due to the higher stability of copper-complexes, Cu^{2+} can displace Zn^{2+}, Fe^{2+} or Ag^{+} ions, and this can be traced by cyclic voltammetry. Consequently, the ferrocenyl ligand makes it possible to detect Cu^{2+} ions even in the presence of other metals.

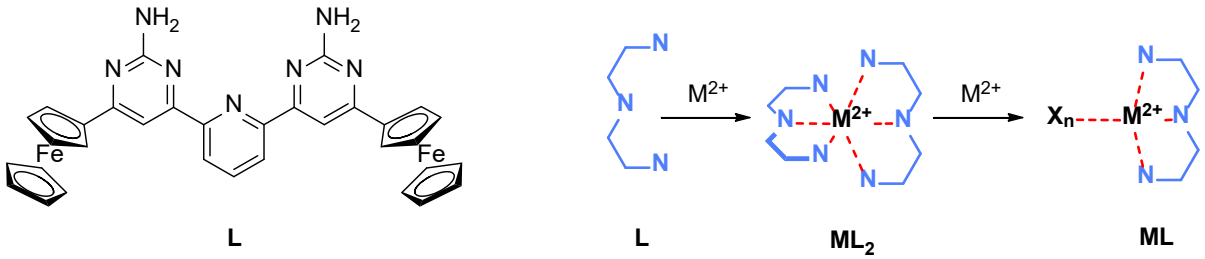

Fig. 1. Ferrocenylpyrimidine ligand **L** and formation of its metal complexes

The financial support of the National Research, Development and Innovation Office (Project: Advanced 149644) is acknowledged.

[1]Kainat, S. F. et al. *RSC Adv*., **2024**, *14*, 21464-21537.
[2]Botha, E. et al. *Inorg. Chim. Acta* **2018**, *482*, 514–521.
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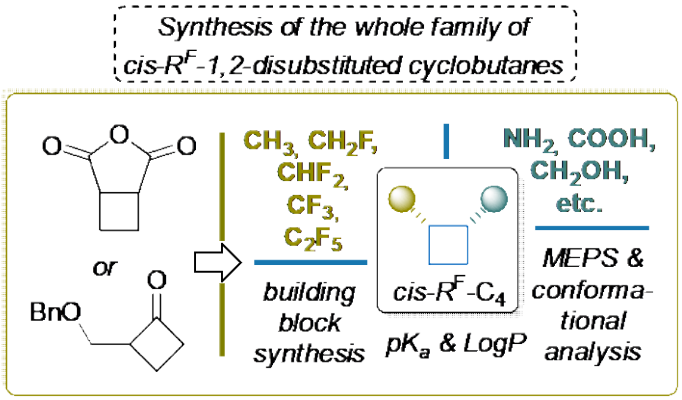
MDR - D1 - P07

Synthesis and physicochemical assessment of *cis*-R^F substituted cyclobutane derivatives

Oleksandr Liashuk[1,2], Anton Chernykh[3,4], Kyrylo Kononenko[3], Artem Michuda[2,3], Oleksandr Olifir[3,5], Serhiy Ryabukhin[1,2,3], Dmytro Volochnyuk[1,3,4], Oleksandr Grygorenko[1,2,3]

[1]Enamine SRI, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Enamine Ltd., Ukraine; [4]Institute of Organic Chemistry NASU, Ukraine; [5]V. P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry NASU, Ukraine

Cyclobutane scaffolds are gaining traction in medicinal chemistry because their rigidity locks substituent vectors in space, enabling tighter control over bioactive conformations. Adding fluoroalkyl groups to these strained rings further broadens their physicochemical space, making them appealing building blocks for drug discovery. Even so, *cis*-1,2-disubstituted cyclobutanes have remained comparatively hard to access, and their properties are much less studied than those of the corresponding *trans* isomers. Here we report an efficient, multigram-scale route to fluoroalkylated *cis*-1,2-disubstituted cyclobutane derivatives. From readily available starting materials, we prepared a diverse series of cyclobutylamines, carboxylic acids, and related compounds in 3–8 steps, on scale up to 39 g. Physicochemical measurements combined with computational analysis uncovered interconnections between conformational effects and observed physicochemical properties, positioning these scaffolds as practical and timely additions to the synthetic toolbox.



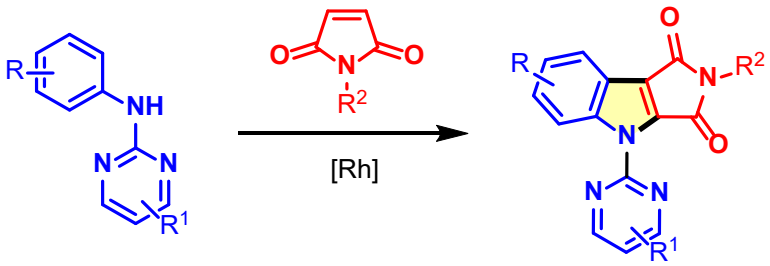
This work was supported by Enamine Ltd. O. Grygorenko and O. Liashuk received additional funding from Ministry of Education and science of Ukraine, grant No. 25BF037-01 (0125U002249).

MDR - D1 - P08

Rh(III)-Catalyzed [3+2] Annulation via C(sp^2)–H Activation for the synthesis of pyrimidinyl-embedded pyrrolo[3,4-*b*]indolediones

Yong Rok Lee[1*], Muhammad Saeed Akhtar[1], Mohammad Aslam[1], Sonaimuthu Mohandoss[1]
[1]*School of Chemical Engineering, Yeungnam University, Republic of Korea*

Indoles constitute a structurally diverse class of compounds with broad biological significance, drawing sustained interest in medicinal chemistry, natural product synthesis, and drug discovery. Ring-fused indoles are widely distributed in nature and exhibit a range of potent biological activities. Among them, pyrrolo[3,4-b]indoles are prominent scaffolds in numerous drugs and bioactive molecules. Despite significant advances in their synthesis, efficient methods for accessing pyrrolo[3,4-b]indolediones remain limited. Herein, we present a facile and efficient Rh-catalyzed strategy for the construction of diversely functionalized pyrimidinyl-incorporated pyrrolo[3,4-b]indolediones from N-arylpyrimidin-2-amines and maleimides via C–H activation/annulation (Scheme 1). In addition, the synthesized compounds exhibit promising potential as fluorescent chemosensors.



Scheme 1

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-00556748).

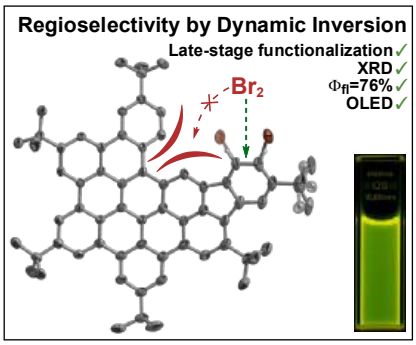
MDR - D1 - P09

OLED material by late-stage functionalization of hexa-*peri*-benzocoronene-fluoranthene hybrid directed by dynamic inversion of helicity

Lina M. Filla[1,+],Alexander R. Krappe[1,+], Jacob C. Mayer[2], Jan M. Sühlo[3], Larissa S. Eitelhuber[1], Anja Wiesner[1], Lukasz Polewski[1], Ute Resch-Genger[4], Beate Paulus[1], Emil J. W. List-Kratochvil[3], Siegfried Eigler*[1]

[1]Freie Universität Berlin, Germany; [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,Germany; [3]Humboldt-Universität zu Berlin, Germany; [4]Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

Nitrile-functionalized emitters suitable for organic light-emitting diodes were accessed via late-stage modification of an asymmetrically distorted hexa-peri-benzocoronene-fluoranthene framework. A regioselective bromination was observed at two peripheral sites, deviating from established electronic and structural expectations that would predict substitution within the K-region. Mechanistic insight from computational analysis indicates that rapid inversion of the helical backbone destabilizes Wheland intermediates at the electronically favoured positions, thereby diverting reactivity to less activated peripheral carbon atoms. Transformation of the brominated intermediates into nitrile-functionalized derivatives yields strongly emissive materials, exhibiting photoluminescence quantum efficiencies of up to 76% in solution. Incorporation of these emitters into multilayer OLED architectures results in luminance values reaching 6,500 $cd \cdot m^{-2}$, enabled by favourable energy-level alignment through appropriate charge-management layers, an effect absent in the corresponding non-functionalized system. Overall, the study highlights how conformational dynamics and broken symmetry can be exploited to steer reactivity and tailor the optoelectronic performance of curved nanographenes.



L. F., A. K., U. R.-G. and S. E. gratefully acknowledge funding from Deutsche Forschungsgemeinschaft (German Research Foundation, Projekt No. 5303118489; grant RE1203/46-1). This work was carried out in the framework of the Joint Lab GEN_FAB and with the support of the Helmholtz Innovation Lab HySPRINT. L. S. E. thanks the German Academic Scholarship Foundation (Studienstiftung des Deutschen Volkes) for their support. We gratefully acknowledge the High-Performance Computing resources of the FUB-IT at Freie Universität Berlin. L. F., A. K. and S. E. would like to acknowledge the assistance of the Cora Facility BioSupraMol supported by the DFG.

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[2]Krappe, A. R.; Mayer, J. C.; Zhang, W.; Filla, L. M.; Ligorio, G.; Hermerschmidt, F.; Eitelhuber, L. S.; Güttler, A.; Weber, M.; Paulus, B.; Resch-Genger, U.; List-Kratochvil, E. J. W.; Eigler, S. *Chem. Eur. J.* **2025**, *31*, e202500742.

MDR - D1 - P10

Enhancing organic electromechemical transistor performance through synthesis of polythiophene wieth carbonyl ester-bridge ethylene glyclol side chains and investigating extended conjugation effects

Y.M. Chen[1], T. Puangniyom[1], H.S. Tseng[2], Y.S. Hsiao[2], and C.C. Chueh[1]*
[1]Dept. of Chemical Engineering, National Taiwan University, Taiwan; [2]Dept. of Materials Science and Engineering, National Taiwan University of Science and Technology, Taiwan

In organic electrochemical transistors (OECTs), conjugated polymers (CPs) facilitate reversible electrochemical reactions during ion implantation, enabling efficient electrical signal amplification. The ion transport properties of these materials are strongly influenced by the molecular design of the polymer side chains. In this presentation, a series of polythiophene (PT)-based CPs with systematically engineered side chains was synthesized to investigate their impacts on electrochemical behavior and thin-film properties—characteristics directly linked to OECT performance. The solid-state structure of CPs containing polyethylene glycol (PEG) side chains was elucidated through X-ray photoelectron spectroscopy (XPS) surface analysis and wettability testing.

The P1 film with branched alkyl-bridged carbonyl ester side chains, the P2 film with tetraethylene glycol-bridged carbonyl ester side chains, and the P3 film containing tetraethylene glycol side chains exhibited distinct ion and electron transport properties. When operating in an aqueous NaCl electrolyte, the P2 film demonstrated enhanced mixed ion/electron transport capabilities and superior long-term stability in OECT operation compared to P3, indicating that ester-linked PEG side chains play a positive role in balancing conductivity and electrochemical robustness. Furthermore, P2 (a backbone-modified derivative) polymer was synthesized using the same method, featuring tetraethylene glycol-bridged carbonyl ester side chains with extended conjugation. The electrochemical properties and film characteristics of P2 were further investigated under mechanical stretching conditions.

The P2 (0T–2T) series is designed to incorporate thiophene units as conjugated spacers between the ester linkage and the conjugated backbone. This spacer design extends the effective conjugation while maintaining the PEG side-chain architecture. Such an approach provides a platform to investigate how conjugation extension adjacent to the backbone influences electrochemical behavior and mixed ion–electron transport. Overall, this study highlights the critical importance of side-chain engineering in tailoring the electrochemical performance, stability, and mechanical adaptability of CP-based materials for advanced OECT applications.

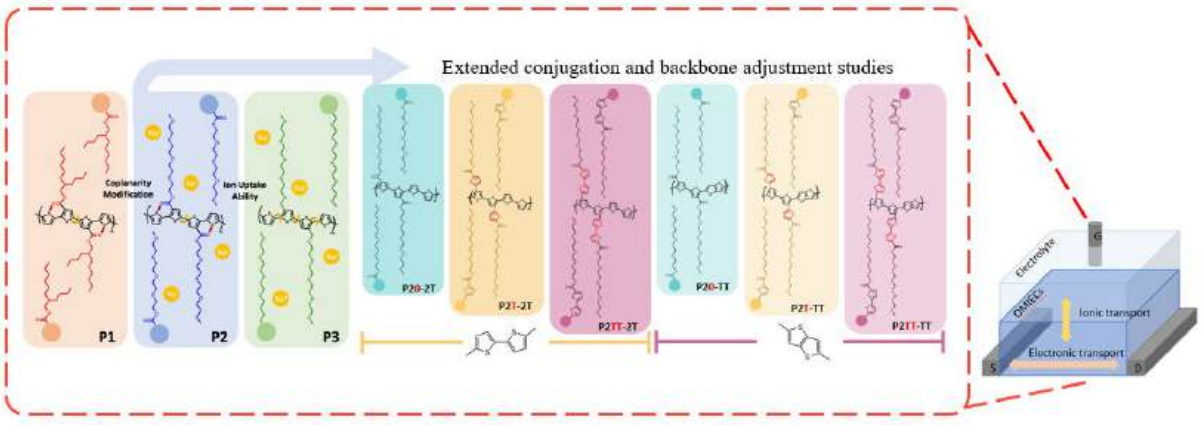

Fig. 1. Overview of side-chain engineering and backbone conjugation strategies in polythiophene-based conjugated polymers for OECT applications. The design integrates PEG side-chain modification, alkyl spacing, and backbone conjugation extension to systematically explore their roles in regulating mixed ion–electron transport.

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MDR - D1 - P11

Synthesis and hosting ability of dynamic *N*-acylhydrazone-based macrocycles

Nicoleta Sandu[1], Anamaria Hanganu[1,2], Codruța Popescu[3], Mihaela Matache[1,4]

[1]University of Bucharest, Faculty of Chemistry, Research Centre of Applied Organic Chemistry, Romania; [2]"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry, Romanian Academy, Romania; [3]University of Bucharest, Faculty of Chemistry, Dept. of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Romania; [4]University of Bucharest, Faculty of Interdisciplinary Studies, Dept. of Interdisciplinary Studies, Romania

***N*-acylhydazones**[1] are versatile molecules due to the reversibility of the hydrazone bond, multiple coordinating sites and the possibility to form hydrogen bonds. These characteristics lead to development of many applications like ligand for coordination compounds[2], synthesis of 2,5-disubstituted-1,3,4-oxadiazoles[3], photoswitching molecules[4], macrocycles[5], dynamic polymers (dynamers)[6] or covalent organic frameworks[7].
We have recently described synthesis of novel [2 + 2] and [3 + 3] ***N*-acylhydrazone**-based macrocycles[8] using a pool of diverse substituted dialdehydes and dihydrazides. The macrocycles were assigned triangular and rectangular shapes. The dimer macrocycle was further assayed for hosting ability using various ions and small molecules. The most intriguing results were obtained using tetra-*n*-butyl ammonium fluoride as studied by NMR and HRMS. Encouraged by these results, we further used other novel dialdehydes and dihydrazides as precursors for ***N*-acylhydrazone**-based macrocycles. We similarly investigated their capacity to host ions or small molecules and we present herein our most recent results. All studies were monitored by NMR and HRMS.

Acknowledgements: This work was supported by a grant from the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1003, within PNCDI III.

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MDR - D1 - P12
Multistate photoswitches containing arylazopyrazole and *N*-acylhydrazones units

George Costache[1,2], Bogdan C. Enache[1,2], Anamaria Hanganu[1,3], Codruța Popescu[1], Anca Păun[1], Augustin M. Mădălan[4], Mihaela Matache[1,5]
[1]University of Bucharest, Faculty of Chemistry, Dept. of Inorganic, Organic Chemistry, Biochemistry and Catalysis, Research Centre of Applied Organic Chemistry, Romania; [2]SC Microsin SRL, Dept. of Research and Development, Romania; [3]Institute of Organic and Supramolecular Chemistry "C.D. Nenițescu" of the Romanian Academy, Romania; [4]University of Bucharest, Faculty of Chemistry, Dept. of Inorganic Chemistry, Romania; [5]Faculty of Interdisciplinary Studies, Dept. of Interdisciplinary Studies, University of Bucharest, Romania

Molecular switches are defined as molecules capable of undergoing reversible transitions between two or more distinct states in response to external stimuli. When the stimulus is light, such compounds are classified as photoswitches. Over the last decades, these systems have attracted significant research interest, as each isomer exhibits distinct physico-chemical properties.[1] The ability to modulate these properties using light at different wavelengths has enabled development of advanced functional materials, including molecular motors, smart photoresponsive polymers, as well as high spaciotemporal control of biological systems[2]. Incorporating multiple photoswitchable moieties within a single molecular scaffold grants access to multiple interconvertible states and this gives rise to materials that can have enhanced properties such as higher capacity for solar thermal fuels and storage data.[3]
Combination can be made using the same switchable unit or mixing different chromophores. In the latter case, the compounds can be selectively addressed with multiple stimuli. A literature survey indicated lack of combination between the azo group and the *N*-acylhydrazone units in the same scaffold. Thus, we designed compounds that combine the robust and great performing arylazopyrazole motif with a series of *N*-acylhydrazones that present the capacity to be locked via metal ion coordination[4]. Herein, we present our results regarding synthesis and dynamics of such compounds acting as multistate photoswitches.

Acknowledgements: This work was partially supported by a grant from UEFISCDI, RO-Swiss Multilateral Academic Projects (MAPS), project number 8ROCH／01/07/2025.

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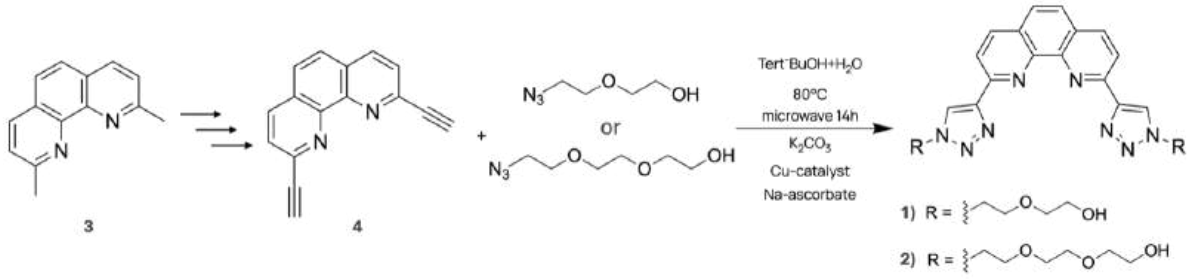
MDR - D1 - P13
Innovative hydrophilic ligands for the selective recovery of Am(III) from spent nuclear fuel

Giulia Marcolli[1,2], Margherita Grieco[1], Massimiliano Federico Silvio Tentorio[1], Giulia De Amicis[1], Elena Macerata[1] and Alessandro Sacchetti[1,2]
[1]Politecnico di Milano, Italy; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy

Managing highly radioactive waste remains a major challenge for the sustainable use of nuclear energy. Currently, spent nuclear fuel (SNF) reprocessing mainly recovers uranium and plutonium for reuse by PUREX (Plutonium Uranium Reduction EXtraction) process, but does little to reduce long-term radiotoxicity. In this perspective, a key difficulty lies in selectively separating americium from curium, two elements with very similar chemical and physical properties[1].The AmSel (Americium Selective Extraction)[2] process seeks to address this issue by selectively removing Am(III) from PUREX raffinate through liquid–liquid extraction.
In this work, we aim to improve the AmSel process by replacing the currently used sulfonated BTBP extractant with new hydrophilic ligands. The proposed extractant must be fully burnable at end of life, composed only of carbon, hydrogen, oxygen, and nitrogen, and capable of selectively extracting americium. The work focuses first on synthesizing the ligands and optimizing their preparation to obtain compounds soluble in acidic aqueous media. Ligands **1** and **2** are based on the phenanthroline scaffold and prepared as shown in Scheme 1. Starting from the oxidation of phenanthroline (compound **3**), and subsequently performing a Seyferth–Gilbert homologation, it is possible to obtain an alkynyl-functionalized phenanthroline. Reaction of this intermediate with *2-(2-azidoethoxy)ethanol* or *2-[2-(2-azidoethoxy)ethoxy)ethanol]* produces ligands **1** and **2**, respectively.
The extraction performance is then evaluated through batch liquid–liquid extraction experiments using radioactive tracers (^{241}Am, ^{244}Cm, and ^{152}Eu) to simulate the target elements present in the SNF. By varying ligand concentration and acidity, optimal operating conditions were identified. The results are encouraging, showing that compounds **1** and **2** are promising alternatives to the reference SO_3-Ph-BTBP extractant, with potential to further enhance the effectiveness of the AmSel process.



Scheme 1. Reactions for the synthesis of the ligands **1** and **2**

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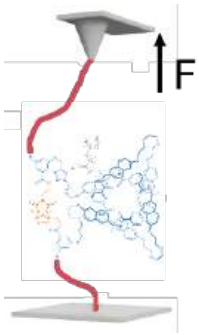
MDR - D1 - P14
Single-molecule force spectroscopy of a trefoil knot gated by a Diels-Alder mechanophore

Martin Blavier[1], Min Zhang[2,3], Robert Nixon[2], Guillaume De Bo[2], David A. Leigh[2,3], Anne-Sophie Duwez[1]
[1]University of Liège, Belgium; [2]University of Manchester, United Kingdom; [3]East China Normal University, China

Molecular knots are ubiquitous in both biological and synthetic materials.[1] The presence of entanglements leads to the reduction of the tensile strength of the material[2], as can be revealed experimentally using single-molecule techniques[3]. This represents an apparent drawback of knotted systems. Knotting also bears some advantages; however, they are not yet fully understood. For proteins, it has been proposed that it might enhance its thermodynamic or mechanical stability.[4]
In the case of synthetic materials, even less is known. A recent single-molecule force spectroscopy study on a small synthetic knot has shown that the knot is able to accommodate mechanical stress and provide a reserve of extensibility.[5] In this study, the metallic coordination centre played an important role in the tightening process and its reversibility. The mechanistic implications of entanglements without a coordinating agent remains unknown.
Here, we use AFM-based Single-Molecule Force Spectroscopy (SMFS) to investigate the mechanical properties of an overhand or trefoil knot gated by a mechanophore built from a furan/maleimide Diels-Alder adduct. This mechanophore allows us to keep the molecular knot loose without a complexing agent. To attach this central portion to the AFM apparatus, a block copolymer of poly(methyl acrylate) (PMA) and poly(glycidyl acrylate) (PGA) linkers is used. The PGA segments allow the creation of strong silicon-epoxide chemical bonds with the tip of the AFM and the surface below, thereby enabling to reach high forces to break the mechanophore made of dynamic covalent bonds.
We report here results on the mechanical response of the gated knot in the form of force-extension curves. In particular, we report patterns providing insight into the rupture mechanism of the mechanophore and the tightening of the knot. We also compare them to patterns observed in the presence of a lutetium complexing agent.



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MDR - D1 - P15
A diastereoselective synthesis of small αα calix[4]pyrrole building blocks

Clara Schritt[†1], Janos Wasternack[†1], Friedrich Braune[1], Sebastian Müller[1], Carlo Fasting[1], Daniel Bombei[1], Siegfried Eigler[1] and Christoph A. Schalley[1]
[1]*Freie Universität Berlin, Germany*

Two-walled αα calix[4]pyrroles are versatile anion- and ion-pair receptors that are used in supramolecular assemblies and functional materials.[1] Their preparation commonly proceeds via the statistical formation of a mixture of αα/ab calix[4]pyrrole diastereomers and subsequent separation of the diastereomers.[2] Since most applications only use the αα diastereomer, the αβ diastereomer usually goes to waste. The chromatographic separation of the statistical mixture of diastereomers is challenging for calix[4]pyrroles with aromatic walls and was not yet reported for calix[4]pyrroles with aliphatic *meso*-substituents.
In this work, we have studied different approaches to the isolation of αα calix[4]pyrroles.[3]
First, the issue of chromatographic separability was addressed. A chromatographic method for the separation of calix[4]pyrrole diastereomers was developed.
To obtain small two-walled αα calix[4]pyrrole building blocks on a synthetically useful scale, we developed a diastereoselective synthesis. Method-optimization led to high yields of αα calix[4]pyrroles. The versatility of the synthesis was demonstrated by the preparation of different targets. Further, methods for chemoselective post-functionalization of those αα calix[4]pyrrole building blocks enable their implementation within functional materials.
With this study, we want to kick start the development of more controlled diastereoselective calixpyrrole syntheses and deliver access to versatile building blocks for complex molecular architectures.

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MDR - D1 - P16

A scalable and resource-saving synthesis of dipyrromethanes and tetrapyrroles - minimal polymer formation and facile purification[1,2]

Janos Wasternack*[1], Clara Schritt[1], Luca Steiner[1], Ole Specht[1], Friedrich Braune[1], Marius Balizs[1], Sebastian Müller[1], Anja Wiesner[1], Beate Paulus[1], Siegfried Eigler[1], Christoph A. Schalley*[1]
[1]Freie Universität Berlin, Institut für Chemie und Biochemie, Germany

Dipyrromethanes and **tetrapyrroles** are important **building blocks** in material sciences, selective adsorbents and filters, medicinal chemistry, bioimaging and photocatalysis with fluorescent dyes and supramolecular chemistry. Their synthesis often is a **bottleneck** in their application, with common hurdles being extensive polymer formation, limited functional group tolerance, low yields and poor scalability.[3,4]
We present an **improved** methodology for the **synthesis** of dipyrromethanes and tetrapyrroles. A key improvement is the drastic **reduction of polymerization** which highly simplifies purification, either by recrystallization or short column chromatography. Also, the **mild conditions** put forth excellent yields and a high functional group tolerance.[1]
Key advantages of the new procedure are: Drastically **reduced consumption** and efficient **recycling** of pyrrole leading to **cost savings**. The new protocols deliver high yields and high-purity products. **Scale-up** preparation of dipyrromethanes was performed on 1000 mmol scale and of tetrapyrroles on 250 mmol scale.
The procedure will be useful in a broad field of **applications within functional materials**, particularly in the emerging field of C[4]P-based materials. Versatile electrophilic and nucleophilic building blocks with **synthetic anchors** were obtained on **multi-gram scale.** In total, **27 dipyrromethanes** and **20 tetrapyrroles** have been prepared, covering a **wide range of functional groups** and reactivity types.

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MDR - D1 - P17

Bicyclic 1,4-dioxepanes - novel advanced building blocks for drug discovery

Bohdan V. Vashchenko[1,2], Illia O. Doroshenko[1,2], Andriy V. Bondarenko[1,3], Oleksandr O. Grygorenko[1,2,3]
[1]Taras Shevchenko National University of Kyiv, Ukraine; [2]Enamine SRI, Ukraine; [3]Enamine Ltd, Ukraine

We report a practical route to saturated fused and spirocyclic 1,4-dioxepane scaffolds designed as multifunctional building blocks for drug discovery. The sequence is based on the construction of the seven-membered ring from vicinal 1,2-diols, followed by alkylative cyclization and functionalization to introduce common building-blocks (primary/secondary amines, carboxylic acids, alcohols). (Figure 1, A).
Measured log*P* and *p*K$_a$ values indicate that the dioxepane scaffolds occupy an intermediate space between morpholine and piperidine analogs (Figure 1, B). A virtual library built from representative amine building blocks was generated and evaluated against common drug- and lead-likeness filters; the majority of members met standard criteria for medicinal chemistry campaigns (Figure 1, C).
Single-crystal X-ray structures of selected representatives were used to perform exit-vector and conformational analyses. These data show that the 1,4-dioxepane-containing bicyclic systems exhibit distinct spatial arrangements of substituents compared to monocyclic analogs and can serve as elongated, slightly distorted surrogates for piperidine-type motifs, while retaining some conformational flexibility (Figure 1, D).

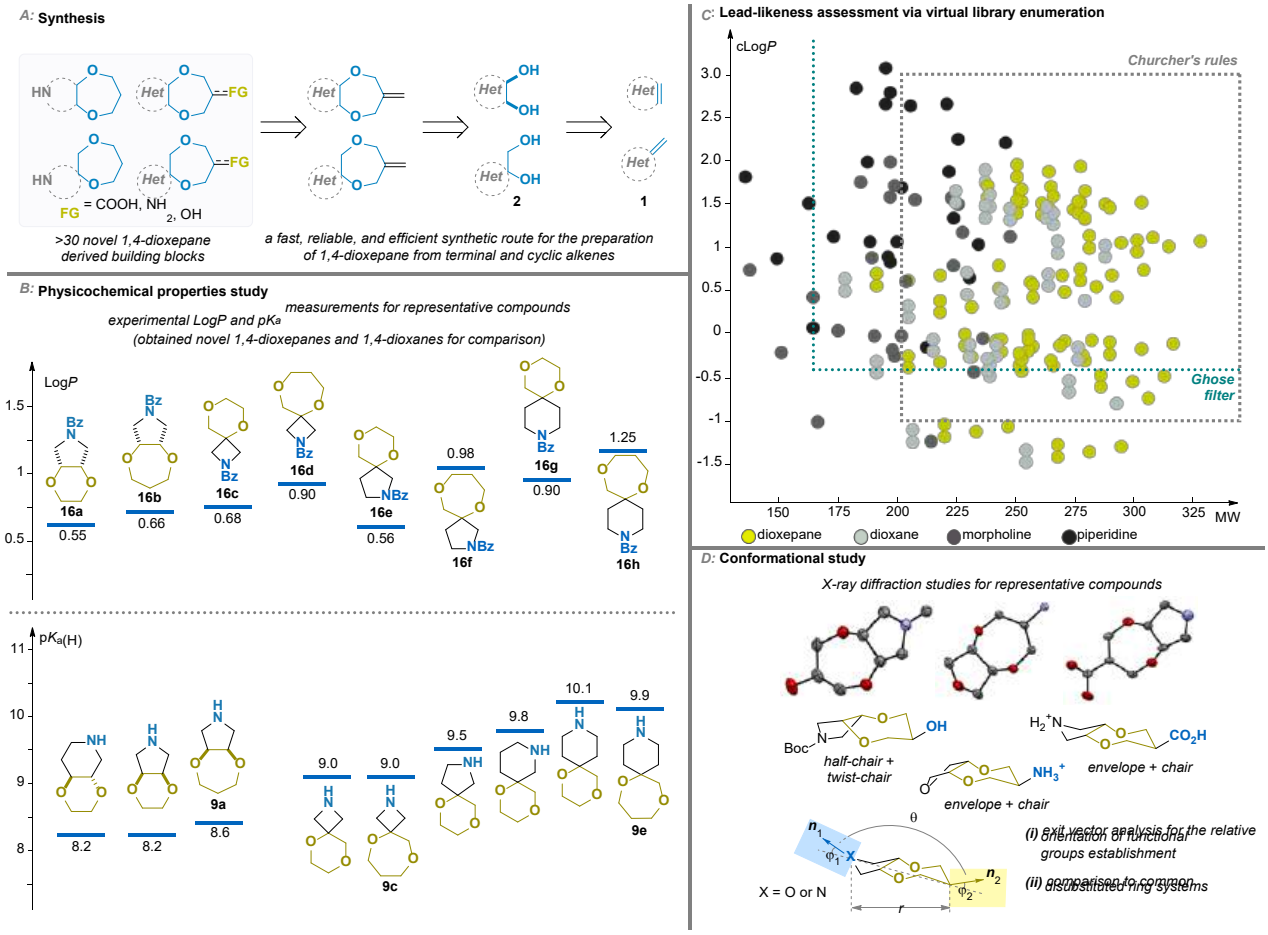

Fig. 1. (A) Retrosynthetic approach to the target saturated bicyclic 1,4-dioxepanes. (B) ORTEP diagrams and conformations of compounds. (C) p*K*$_a$(H) and Log*P* values for compounds. (D) MW – cLog*P* plot of the generated virtual library.

MDR - D1 - P18
Stability of heteroaromatic sulfonyl chlorides and fluorides

Bohdan V. Vashchenko[1,2], Illia O. Doroshenko[1,2], Oleksandr I. Shevchuk[1,3], Oleksandr O. Grygorenko[1,2,3]
[1]Taras Shevchenko National University of Kyiv, Ukraine; [2]Enamine SRI, Ukraine; [3]Enamine Ltd, Ukraine

Heteroaromatic sulfonyl halides are key building blocks for the synthesis of sulfonamides and related motifs, yet their practical use is often limited by insufficiently understood stability issues. In this work, we present a comprehensive experimental analysis of structure–stability relationships across a large and diverse set of heteroaromatic sulfonyl chlorides and fluorides (Figure 1, A).
A total of 236 synthesized sulfonyl halides (165 of them were prepared for the first time) were examined under both solution and neat storage conditions over extended periods. Stability trends were correlated with heterocycle type, substitution pattern, and the nature of the halide. Sulfonyl chlorides were found to undergo decomposition primarily via SO_2 extrusion or hydrolysis (Figure 1, B), with pronounced dependence on the position of the sulfonyl group and the electronic and steric properties of substituents. Sulfonyl fluorides were generally significantly more stable across all series.
Based on these data, practical guidelines are proposed to assist chemists in selecting between sulfonyl chlorides and sulfonyl fluorides for specific heteroaromatic scaffolds (Figure 1, C). The results provide an empirical framework for improving reagent choice, storage, and reliability in medicinal chemistry and related synthetic applications.

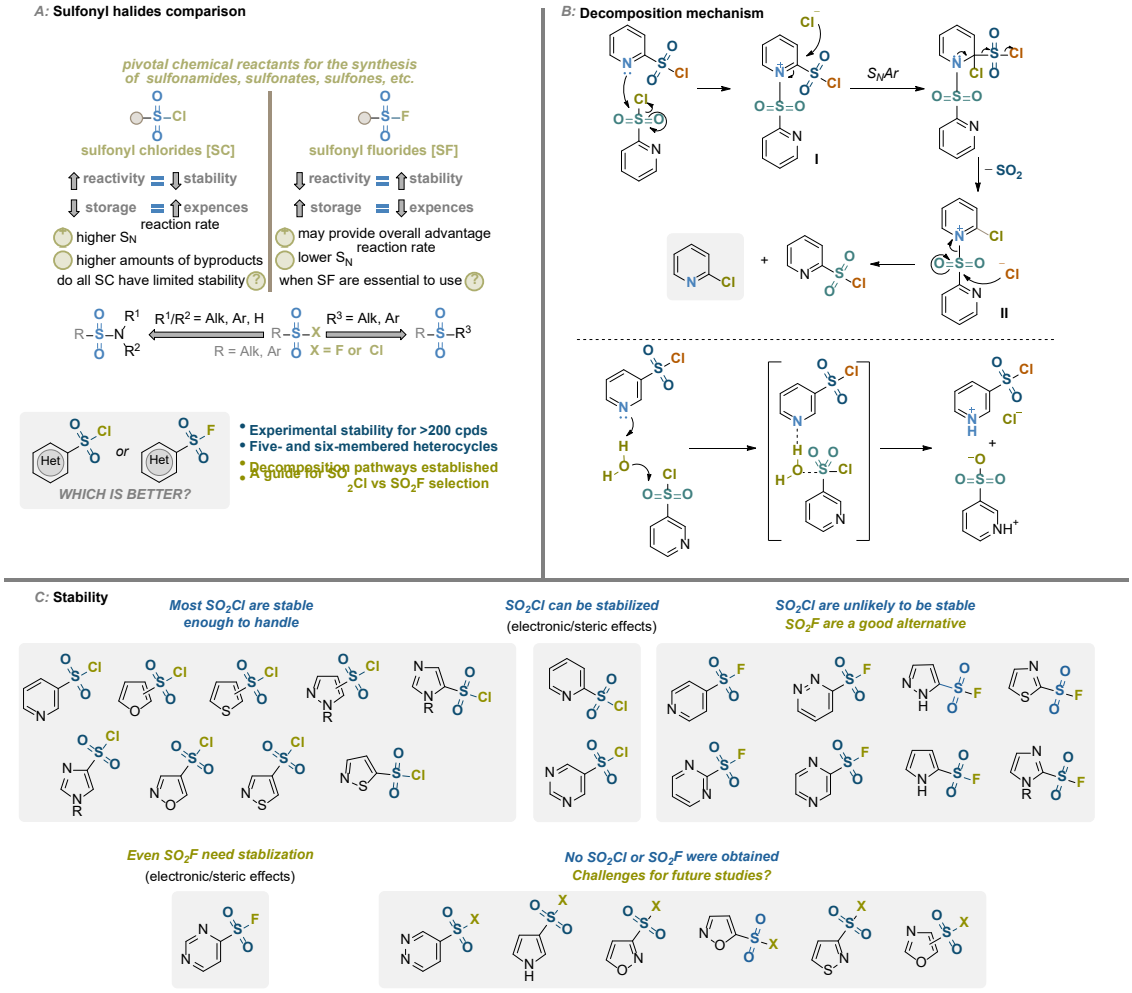

Fig. 1. (A) Sulfonyl chlorides versus sulfonyl fluorides. (B) A proposed mechanism for the decomposition of sulfonyl chloride compounds. (C) Stability guidelines for heterocyclic sulfonyl halides (chlorides *vs* fluorides).

MDR - D1 - P19

Novel 2-pyridl functionalized thiazolo[5,4-*c*]isoquinolines as selective chemosensors for metal cations

Letícia D. Costa[1,*], Nuno M. Moura[1], Amparo F. Faustino[1], Augusto C. Tomé[1]
[1]LAQV-REQUIMTE, Dept. of Chemistry, University of Aveiro, Portugal

Metal ions are essential for living systems, playing an essential role in several biochemical processes. However, due to their intrinsic toxicity and persistence in the environment, their concentration must be tightly monitored both in biological and environmental systems.[1–3] The design and synthesis of optical probes for analyte recognition have become increasingly significant due to the cost-effectiveness and versatility of spectrophotometric and spectrofluorimetric techniques. Effective chemosensors must incorporate a selective recognition site with a measurable change in absorption or fluorescence. Fluorophores are particularly valuable for ion quantification. The development of these devices relies on optimizing key criteria, including chemical stability, metal affinity, selectivity, rapid signal transduction, and overall accessibility.[4] Therefore, due to their high sensitivity, selectivity and fast response, in particular when compared with conventional analytical methods, the development of new chemosensors for metal ion recognition has emerged as a prominent research field.[5]

Thiazolo[5,4-*c*]isoquinolines (TzIQ) were first synthesized several years ago, but it was only recently that the study of its properties and applications was deepened.[6] In this communication we report the synthesis of two new thiazolo[5,4-*c*]isoquinoline derivatives, obtained via Suzuki–Miyaura cross-coupling with pyridin-2-ylboronic acid. The photophysical properties and the sensing ability of these compounds towards a range of metal cations will be discussed. The outstanding enhancement in the fluorescence emission observed for one of these TzIQ derivatives in the presence of Cu^{2+} (**Figure 1**) will be also discussed.

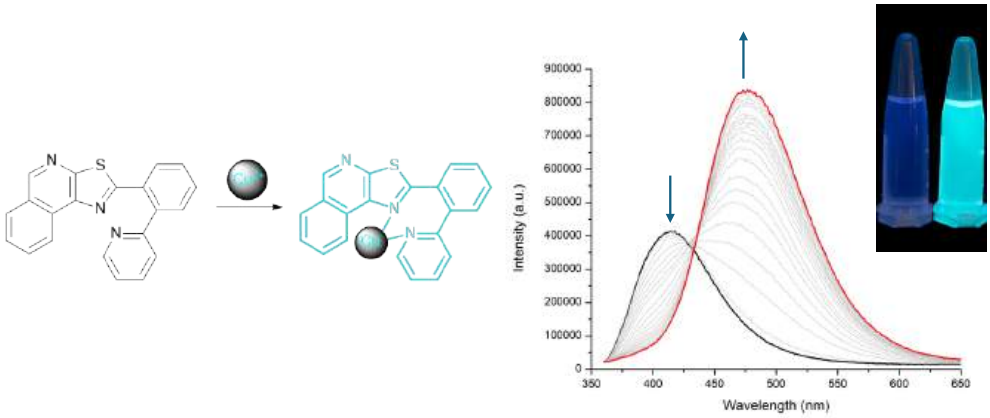

Fig. 1. Increased fluorescence emission of TzIQ in the presence of Cu^{2+}.

This research work received financial support from the University of Aveiro and FCT/MCTES to support UID/50006/2025-Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos research unit. NMM Moura gratefully acknowledges FCT for an Assistant Research Position under the Individual Scientific Employment Stimulus - 6th Edition (2023.06495.CEECIND/CP2840/CT0031; DOI: 10.54499/2023.06495.CEECIND/CP2840/CT0031).

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MDR - D1 - P20
Difluromethoxy group as a new MedChem handle

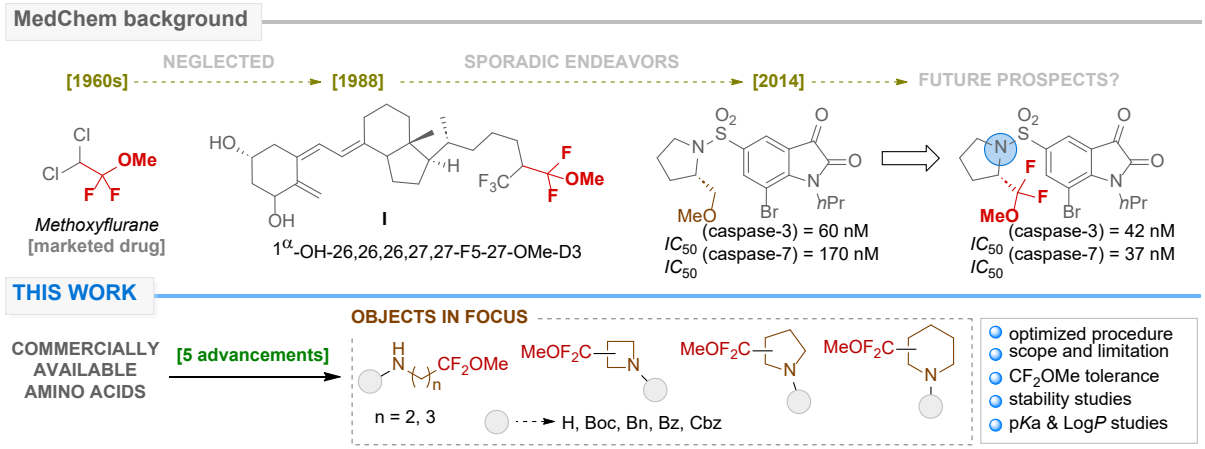
Mykhailo Pashko[1,2], Dmytro Granat[1,3], Oleksii Klymenko-Ulianov[1], Dmytro Leha[3,4], Serhiy Ryabukhin[1,2,3,4], Dmytro Volochnyuk[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Institute of Organic Chemistry, Ukraine; [3]Taras Shevchenko National University of Kyiv, Ukraine; [4]Enamine Scientific Research Institute, Ukraine

Fluorination has become a routine strategy for modulating potency, selectivity, and ADMET properties in contemporary medicinal chemistry. As the field gradually shifts from aromatic fluorination toward more three-dimensional and metabolically robust aliphatic motifs, access to unconventional fluorinated fragments becomes a defining bottleneck. One of the most promising, yet curiously underexplored, substituents is the difluoro(methoxy)methyl (CF_2OMe) group. The literature provides solid evidence that it is an attractive but rarely implemented motif in practice. This is largely because reliable building blocks and scalable synthetic entry points remain limited.

In this report, we aimed to convert CF_2OMe from an “interesting idea” into a routine MedChem handle. We developed a modular, operationally straightforward platform for preparing CF_2OMe-containing amines. Importantly, the study was designed not merely as a substrate scope exercise, but as a methodology-driven analysis identifying the key factors governing success and reproducibility.

A central enabling element is an imidate-based thionation strategy that delivers diverse thionoesters from both cyclic and acyclic amines, thereby establishing a scalable entry to the fluorination step. Systematic reaction mapping revealed structure-dependent performance trends and practical constraints (including protecting-group effects, steric sensitivity, and side-product formation), enabling the formulation of clear selection rules for substrate design and reaction success.

Beyond synthesis, we demonstrate that CF_2OMe amines can be integrated into medicinal chemistry workflows via common transformations, including protection/deprotection, acylation, amide coupling reactions, and N-arylation. Physicochemical profiling revealed that CF_2OMe occupies a distinct region in LogP-pKa(H) space, enabling the predictable, simultaneous tuning of lipophilicity and basicity relative to common fluorinated substituents. Finally, the high chemical and biostability of CF_2OMe further support its attractiveness for MedChem and agrochemical applications.



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MDR - D1 - P21

Synthesis and characterization of the silver (I) tranexamate complex with potential antibacterial activity

Guillermo José Gallardo Vásquez[1], Milca Yeni Choque Diaz[1]
[1]*Farmacia Magistral JPG SKIN, Peru*

Bacterial infections affect the normal course of wound healing in burn patients, leading to high mortality rates. It is estimated that 180,000 deaths occur each year, representing 75%, which makes developing new antibacterials that act as bactericides or bacteriostatic agents a significant challenge. Current conventional therapies have many limitations, one of them being bacterial resistance, which is why there is a need to synthesize new broad-spectrum antimicrobials. The study was carried out in two phases; the first consisted of the synthesis and characterization of Silver Tranexamate. For this, we mixed aqueous solutions of tranexamic acid and sodium hydroxide, 0.005 mol each, stirred for 30 minutes, and then gradually added an aqueous solution of silver nitrate, 0.005 mol; after 1 hour of stirring in a tightly closed container, a whitish solution was obtained; it was filtered by gravity, washed with cold anhydrous ethanol, and placed in an oven at 30 °C for 5 hours. A white powder was obtained. The reaction yield was 65%. For characterization, the following tests were performed: FTIR spectroscopy (Fig.1), Nuclear Magnetic Resonance, Elemental Analysis, and Thermogravimetric Analysis. In the second phase, o/w creams based on the synthesized complex were prepared at concentrations of 0.25%, 0.5%, 1%, and 2%. The Kirby Bauer method (Fig. 2) was conducted to determine the antibacterial effect of the creams against *Staphylococcus aureus*. Statistical tests such as Levene, ANOVA, and Tukey were used to identify statistical differences among the different concentrations. The complex was synthesized, and it was determined that the 2% o/w cream showed the best antibacterial effect (13.7850 mm) with a 95% confidence level and a 0.05% error rate. Future research could be carried out with other present bacteria and in burn wounds.

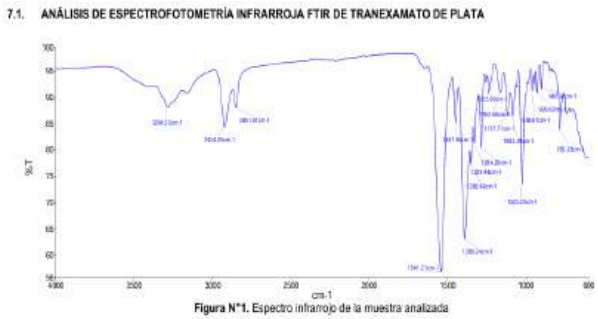

Fig.1. FTIR Analysis of Silver Tranexamate

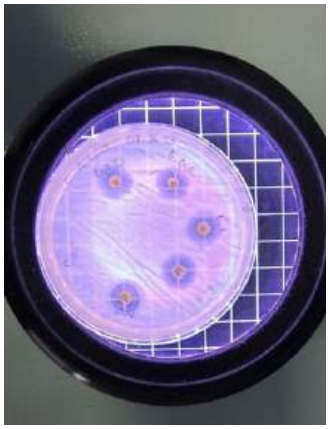

Fig. 2. Antibacterial Activity against Staphylococcus aureus

Acknowledgments: Dr. José Fabián Schneider, NMR Laboratory, Institute of Physics of São Carlos, University of São Paulo.

MDR - D1 - P22

Synthesis of diverse allylic sulfone derivatives via sequential hydroxylation of 1,3-enynes

Sourav Kumar[1], Bhahwal Ali Shah[2], Indrajit Ghosh[1], Radek Zboril[1]
[1]VSB - Technical University of Ostrava, Czech Republic; [2]CSIR-Indian Institute of Integrative Medicine, India

A first metal-free protocol for the synthesis of allylic sulfones featuring aldehyde functionality at the δ-position has been reported. The formation of structurally complex δ,δ-dimethoxy allylic sulfones is enabled by the direct nucleophilic attack of methoxide onto the sulfone-containing 1,3-enynes. The present approach allows facile installation of acetal groups within the allylic sulfone scaffold, providing versatile platforms for further functionalization and drug development.

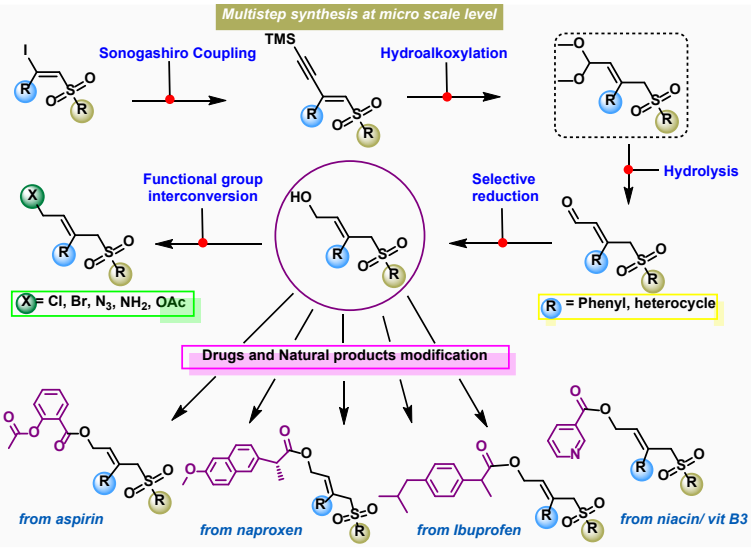

Fig. 1. Synthesis of Diverse Allylic Sulfone Derivatives.

S.K. acknowledges the financial support of the European Union under the REFRESH – Research Excellence for REgion Sustainability and High-tech Industries project number CZ.10.03.01/00/22_003/0000048. B.A.S. gratefully acknowledge SERB, Dept. of Science and Technology (DST), Govt. of India for financial assistance (000850/2021).

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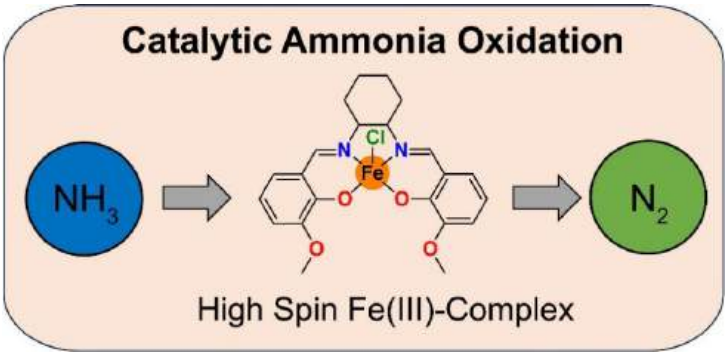
MDR - D1 - P27

Catalytic ammonia oxidation mediated by high-spin Fe(III) complex: Combined experimental and DFT study

Mohammad Usman[1], M. Nasiruzzaman Shaikh*[1]

[1]Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia

Ammonia offers high hydrogen density and favorable transport properties, making it an appealing hydrogen carrier; yet conventional cracking methods for hydrogen release are energy-intensive. Molecular iron complexes offer a sustainable route for the homogeneous conversion of NH_3 to N_2 under mild conditions. Here, we describe a high-spin FeIII-complex bearing a tetradentate *N,N,O,O*-donor trans-1,2-bis(2-hydroxy-3-methoxyphenyl-methaniminyl)cyclohexane ligand framework that catalyzes ammonia oxidation at room temperature. In combination with a triarylaminium oxidant and 2,4,6-collidine base, the catalyst produces up to 2.20 equivalents of N_2 per Fe center. Comprehensive characterization of the Fe^{III}-complex by FTIR, UV-vis, XPS, and X-ray diffraction, with Mössbauer and DFT analysis, confirmed its high-spin state. Moreover, DFT studies revealed that N–N bond formation in ammonia oxidation proceeds through nucleophilic attack followed by sequential proton- and electron-transfer steps. Together, these findings underscore the potential of high-spin Fe^{III}-complexes in ammonia oxidation catalysis and provide crucial mechanistic understanding of N–N bond formation.



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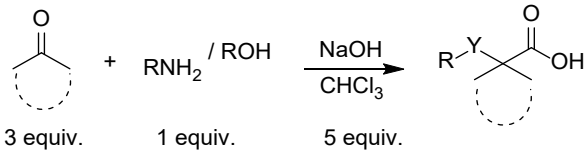
MDR - D2 - P01

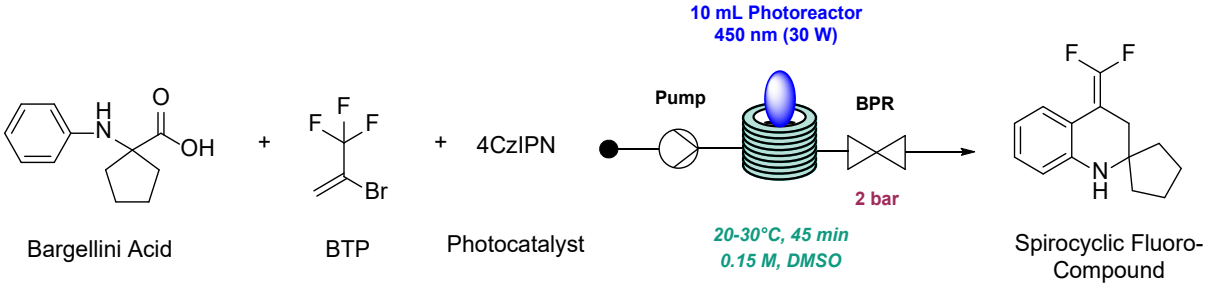
Development of continuous flow photocatalytic decarboxylative cross-coupling reactions of bargellini acids

Lee Chieng[1], Marcus Baumann[2]
[1]University College Dublin, Ireland; [2]University College Dublin, Ireland

The Bargellini reaction is an organic transformation first reported by Guido Bargellini in the early 20th century. [1] The reaction attracted attention for its ability to construct densely functionalised molecules from relatively simple starting materials. Its discovery provided a new route for the formation of sterically hindered α-substituted carboxylic acids and related compounds in a one-pot fashion. [2]



The synthesis of spirocyclic fluoro-compounds was successfully achieved using continuous flow photochemistry based on the Bargellini acids. [3] The photocatalytic decarboxylation Giese reaction was performed utilising the organic dye 4CzIPN as a photocatalyst. [4] The novel spirocyclic fluoro-scaffolds has many interesting features in medicinal chemistry, such as the incorporation of the fluorine, the spirocyclic framework and the tetrahydroquinoline core. The spirocyclic fluoro-scaffolds will be further derivatised for different applications. [5-6]



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MDR - D2 - P02
Exploiting flow technology for the sustainable synthesis of industrially relevant building blocks

Dylan Mangru,[1] Danielle Curran,[2] Pat O'Neill,[2] and Marcus Baumann.[1]
[2]*University College Dublin, Ireland;* [2]*Pfizer, Ireland*

Utilising simple chemical building blocks that can be ultimately derived from carbon dioxide, formaldehyde and glyoxal is attractive to synthesise novel poly-oxygenated heterocycles.[1] For instance, the bent structure of such bicyclic dioxanes should give a steric hindrance to S_N2 attack.[2] Utilising other aldehydes and ketones, photochlorinations, photocatalysis, and carbenes, were investigated to derivatise the heterocycles.
These heterocycles can be substituted at either the acetal or bridgehead sites using radical, carbene or anionic chemistry to functionalise the molecule. Derivatisation with highly reactive intermediates makes continuous flow chemistry an ideal method to investigate the reactivity of these molecules.

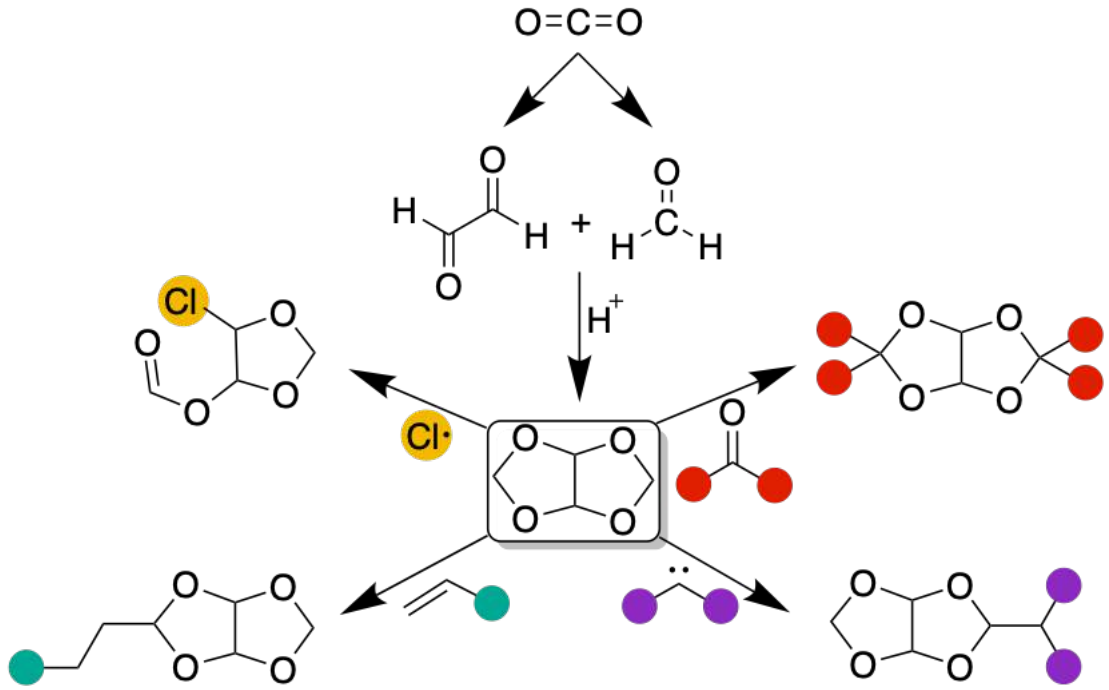

Fig 1. Formation of novel polyoxygenated heterocycles and their derivatisations.

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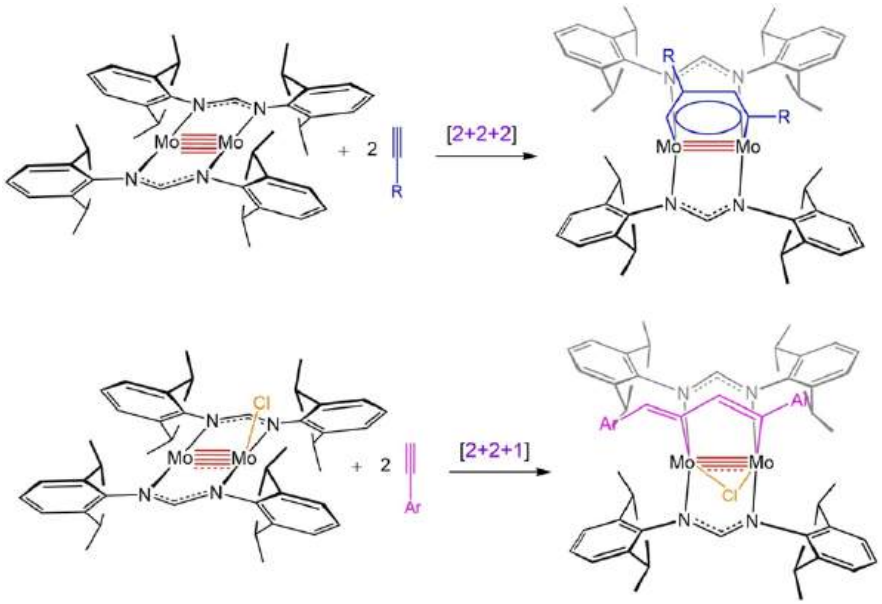
MDR - D2 – P03
Extending [2+2+2] and [2+2+1] cyclizations to mo–mo and w–w multiply bonded complexes

Yi-Chou Tsai
Dept. of Chemistry, National Tsing Hua University, Hsinchu, Taiwan

[2+2+2] and [2+2+1] cycloaddition reactions are well-established synthetic tools in organic chemistry for the construction of cyclic frameworks.[1,2] In this presentation, I will describe our recent work extending these cyclization strategies to multiply bonded Mo–Mo and W–W complexes. We have discovered that two equivalents of terminal alkynes react with N-donor-supported Mo–Mo[3] or W–W complexes to form six-membered[3] and five-membered metallocycles that retain an intact metal–metal multiple bond within the ring. Comprehensive spectroscopic and single-crystal X-ray diffraction studies reveal that these unprecedented metallocycles display pronounced aromatic character, arising from the incorporation of metal–metal bonding interactions into the cyclic π framework. This chemistry expands the scope of conventional cycloaddition reactions by integrating metal–metal multiple bonds as active participants in ring construction. Moreover, it provides a versatile and modular approach to the synthesis of aromatic metallocycles with potential relevance to catalysis and functional materials. The presentation will cover reaction development, mechanistic considerations, and the structural and electronic properties of these unique metal-containing aromatic systems.



Financial support from the National Science and Technology Council (NSTC), Taiwan (Grant Nos. 111-2113-M-007-012-MY3, 114-2113-M-007-013, 114-2113-M-007-008) and National Tsing Hua University is gratefully acknowledged.

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MDR - D2 - P04

[2.2]-to-[3.2] Skeletal editing of the paracyclophane core via controlled phenonium ion formation

Tilman Köhler[1], Andreas Rapp[1], Olaf Fuhr[2], Joachim Podlech[1] , Stefan Bräse[1,3]
[1]Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [2]Institute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [3]Institute of Biological and Chemical Systems – Functional Molecular Systems (IBCS-FMS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany.

Mixed-bridge paracyclophanes (pCp) such as [3.2]paracyclophanes represent structurally unique π-systems with potential applications in ligand design, stereochemically defined architectures, and functional materials. In contrast to the [2.2]pCp topology, their broader use has been limited by the lack of general and direct synthetic access.[1,2] We present a skeletal editing strategy that enables the efficient conversion of readily available [2.2]paracyclophanes into [3.2]paracyclophane frameworks via a highly strained, paracyclophane-derived phenonium ion.

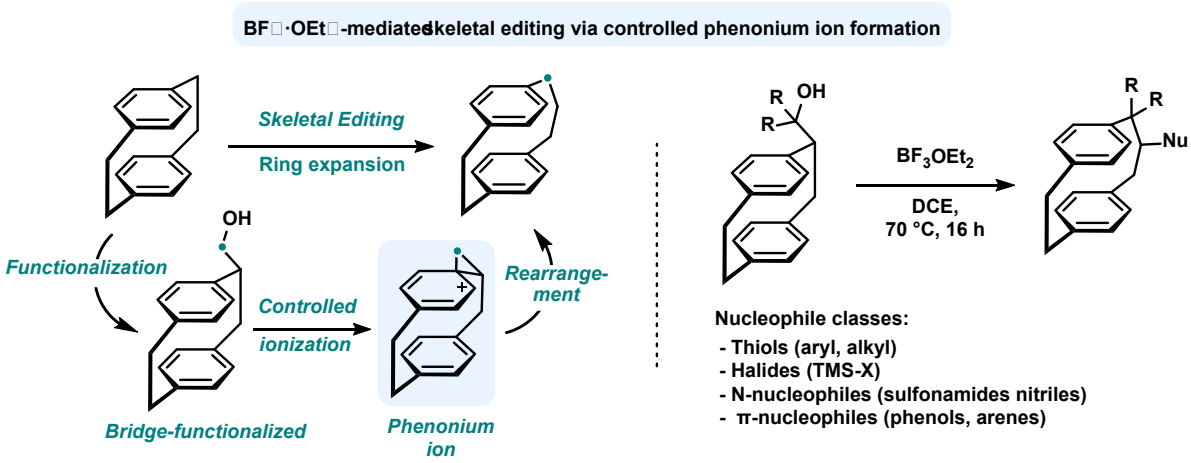

Fig. 2. Skeletal editing of [2.2]paracyclophanes to [3.2]paracyclophanes via controlled phenonium ion formation.

Phenonium ions are promising but underdeveloped platforms for synthetic transformations.[3] This work addresses how the reactivity of this distinctive pCp-derived phenonium intermediate can be controlled and synthetically harnessed. Central to this is the generation of the cation through Lewis-acid-mediated direct alcohol activation, which enables controlled ionization without unselective solvolysis, elimination or degradation. $BF_3{\cdot}OEt_2$ emerged as a uniquely effective activator, and reaction selectivity is governed by efficient interception of the phenonium intermediate by external nucleophiles that must outcompete rapid self-trapping pathways leading to oligomeric material.
Under the optimized conditions, a broad range of sulfur nucleophiles, including aryl, aliphatic, cyclic, and benzylic thiols, afford the corresponding [3.2]paracyclophane derivatives in good to excellent yields. Halogenated products are accessible via silylated halide nucleophiles, and additional trapping modes include sulfonamides and nitriles via a Ritter-type process. The resulting products provide versatile entry points for downstream functionalization at the expanded bridge, enabling further derivatization and access to structurally diverse [3.2]paracyclophane scaffolds.
Mechanistic investigations, including in situ ^1H NMR monitoring, reveal extended zero-order kinetics consistent with rate-determining ionization from a rapidly equilibrating activated complex and fast cation interception. Overall, this work establishes phenonium ions as versatile intermediates for skeletal editing of highly strained architectures and provides a modular and operationally simple entry into [3.2]paracyclophane chemical space.

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MDR - D2 - P05

Synthesis of Amino-functionalized ferrioxamine E biomimetics – Toward modular trihydroxamate macrocycles for late-stage diversification

Adam Włodarczyk[1], Radosław Tymoszewicz-Gaida[2], Elżbieta Wojaczyńska[2,*] and Elżbieta Gumienna-Kontecka[1,*]

[1]Faculty of Chemistry, University of Wrocław, Wrocław, Poland; [2]Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland

Siderophore-inspired hydroxamate macrocycles are attractive scaffolds for radiometal coordination and for the development of pathogen-targeted imaging agents, particularly using ^{68}Ga in PET. [1-4] Recent work on biomimetics based on ferrioxamine E/desferrioxamine E (FOXE/DFOE) shows that subtle structural modifications can tune biological recognition and imaging-relevant properties.

We report the design and synthetic preparation of amino-functionalized FOXE biomimetics that integrate a trihydroxamate metal-binding domain with an orthogonal amine handle enabling downstream conjugation and comparative structure-property studies.

A modular assembly strategy was applied to introduce the amine functionality within the linker region while maintaining the overall hydroxamate architecture. The resulting scaffold family provides a practical entry to bifunctional siderophore-mimetic macrocycles for subsequent derivatization and evaluation in radiolabelling and biological targeting workflows relevant to infection imaging.

The financial support from the National Science Centre of Poland is gratefully acknowledged (grant no. UMO-2022/47/I/ST4/02354).

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MDR - D2 - P07

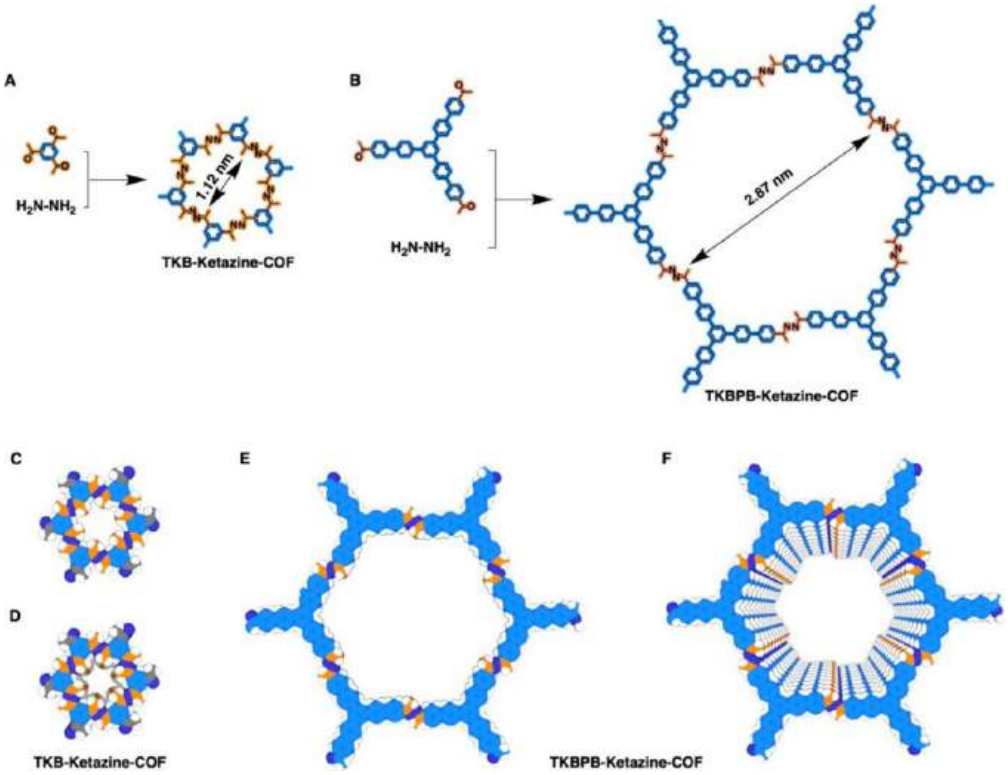
Ketazine-linked covalent organic frameworks: A new linkage platform for crystalline π-conjugated porous materials

Xinyu Mu[1,2], Shuailei Xie[1,2], Xingyao Ye[1,2], Shanshan Tao[1], Juan Li[3], Donglin Jiang[1,2]*
[1]Dept. of Chemistry, Faulty of Science, National University of Singapore, Singapore, Singapore; [2]Joint School of National University of Singapore and Tianjin University, International Campus of Tianjin University, Binhai New City, Fuzhou, China; [3]Institute of Crystalline Materials, Shanxi University, Taiyuan, China

Covalent organic frameworks (COFs) are modular porous materials whose crystallinity and functionality critically depend on the reactivity and electronic nature of the building blocks. However, COF synthesis has been largely restricted to aldehyde-based monomers, while ketone-based monomers have been rarely explored in COF synthesis due to their distinct reactivity. Here, we introduce methyl-substituted ketones as a distinct class of monomers to construct the first ketazine-linked COFs via polycondensation with hydrazine. The methyl substitution modulates the steric and electronic environment of the carbonyl groups, effectively moderating their reactivity and enhancing the reversibility of framework formation, which is essential for achieving high crystallinity.

Through systematic optimization of reaction conditions, highly crystalline two-dimensional COFs with tunable micro- and mesoporosity were reproducibly obtained. Powder X-ray diffraction combined with structural modeling reveals well-ordered hexagonal frameworks adopting eclipsed AA stacking. Beyond crystallization control, alkyl substitution subtly fine-tunes the electronic structure of the π-conjugated backbone, leading to enhanced light absorption and strong blue fluorescence emission in exfoliated COF dispersions. The resulting frameworks further exhibit excellent thermal and chemical stability.

By integrating reactivity modulation and electronic fine-tuning into monomer design, this work establishes a general materials design strategy for constructing π-conjugated porous frameworks with tailored structural order and photophysical properties.



Scheme 1. (A, B) Schematic of the Synthesis of Ketazine-Linked (A) Microporous TKB-Ketazine-COF and (B) Mesoporous TKBPB-Ketazine-COF; (C, D) Reconstructed Crystal Structure of (C) Single Layer and (D) Ten Layers of TKB-Ketazine-COF at Top View. (E, F) Reconstructed Crystal Structure of (E) Single Layer and (F) Ten Layers of TKBPB-Ketazine-COF at Top View (in Parts C–F, C = Blue, N = Orange, and White = H)

MDR - D2 - P08
Topochemical polymerization as a pathway to structurally precise 2D organic polymers

Javed Pathan, Kristof Van Hecke
Ghent University, Belgium

Organic polymers are integral to modern life, forming the foundation of materials used in packaging, textiles, coatings, electronics, and energy technologies. Covalent organic polymers are classified as one-dimensional (1D) or two-dimensional (2D) macromolecules, in which monomer units are covalently linked along one or two axes, respectively.[1] Although conventional solution- or melt-based polymerization strategies have enabled the formation of polymeric sheets, these approaches often suffer from limited crystallinity, the presence of defects, and structural ambiguity, thereby restricting precise structural characterization and rational materials design.[2]
Topochemical polymerization provides a compelling solid-state route to highly ordered 1D and few 2D polymers, preserving single-crystal integrity and enabling atomic-level structural resolution, thereby addressing the intrinsic disorder of conventional polymeric materials. [3] Concurrently, there is a growing interest in 2D polymers owing to their distinctive features, including high surface area, intrinsic porosity, and enhanced mechanical robustness.[4]
We aim to synthesize photoinduced 2D polymers via topochemical reactions, emphasizing reversible polymerization that enables controlled interconversion between 2D and 1D polymeric states while imparting advanced structural and functional properties. In parallel, we design monomers capable not only of undergoing reversible 1D↔2D transformations but also of programmed chain cleavage, allowing access to degradable systems and the generation of entirely new polymer architectures beyond obtained1D and 2D polymers. Overall, this work positions topochemical polymerization as a powerful bridge between polymer chemistry and crystalline materials science for designing precise, stimuli-responsive 2D polymers.

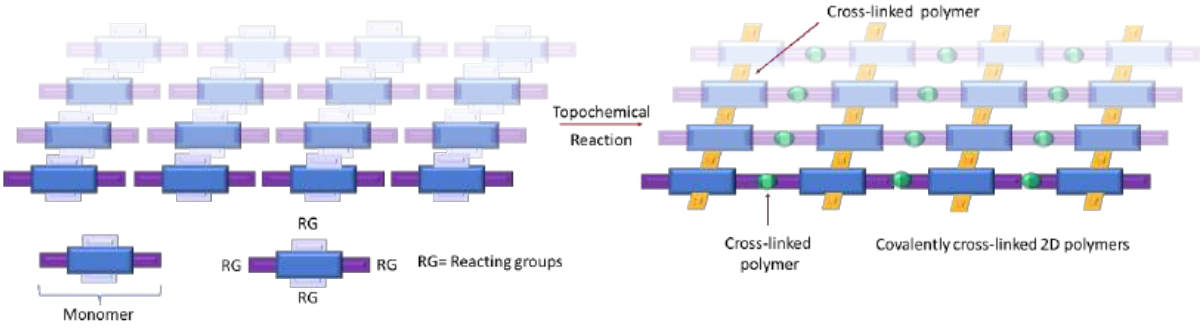


Fig. 1. Schematic representation of covalently linked 2D polymers via topochemical reactions

Acknowledgment: JP and KVH thank the Special Research Fund (BOF) – UGent (Project: bof/baf/4y/2024/01/214).

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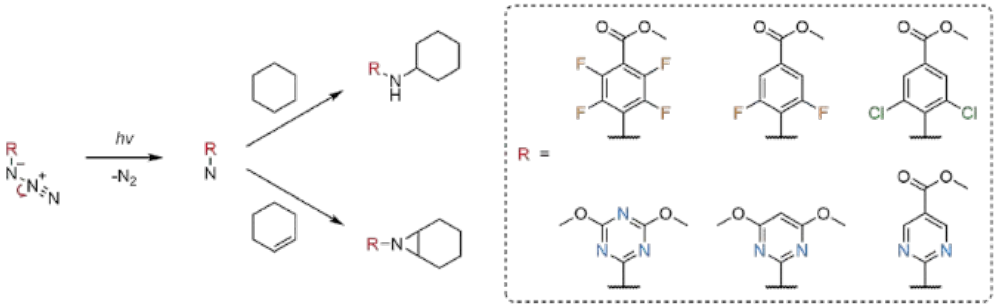
MDR - D2 - P09
Fluorine-free nitrene insertion for covalent functionalization of cross-country skis

Silje Iren Strøm, Audun Formo Buene
Norwegian University of Science and Technology, Norway

Molecular interactions between the ski base and snow are a key factor in determining ski–snow friction. Traditionally, the surface chemistry of ski bases is manipulated using paraffin-based waxes, which adhere to the skis through weak intermolecular forces. To improve the abrasion resistance of glide waxes, we aim to develop a method for modification of ski bases that covalently attaches friction-reducing functionalities to the surface. Modern ski bases typically consist of polyethylene and are therefore inert toward most chemical reagents. A viable approach for covalent functionalization of ski bases is nitrene C-H insertion through decomposition of aryl azides, which has previously been used to introduce perfluoroalkyl chains to skis.[1] Nitrenes derived from fluorinated aryl azides were employed due to their significantly slower intramolecular cyclization and ring expansion compared to unsubstituted aryl nitrenes.[2] However, the recent fluorine ban in competitive skiing renders fluorinated azides inapplicable. Nitrogen-containing heteroaryl scaffolds have emerged as a promising alternative, and nitrene insertion into polyethylene has recently been demonstrated by thermolysis of azido-1,3,5-triazine.[3]
In this work, a selection of fluorinated, non-fluorinated, and heteroaryl azides were synthesized. Nitrene reactivity was compared by studying product distributions and kinetic aspects of their photoinitiated reactions with cyclohexane and cyclohexene. These model reactions confirmed the promising reactivity of heteroaryl azides, encouraging further exploration of their use in polyethylene surface functionalization.



Scheme 3. Model reactions of the investigated nitrene scaffolds.

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MDR - D2 – P10
New heterometallic 4*f*-4*f'* complexes – An original synthetic approach

Diana-Ioana Eftemie[1,2], Sergiu Shova[3], Teodora Mocanu[4], Ingrid Freuze[5], Daniel Avram[6], Carmen Tiseanu[6], Marius Andruh[1,2]
[1]"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry of the Romanian Academy, Bucharest, Romania; [2]University of Bucharest, Faculty of Chemistry, Bucharest, Romania; [3]"Petru Poni" Institute of Macromolecular Chemistry of the Romanian Academy, Iasi, Romania; [4]"Ilie Murgulescu" Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania; [5] University of Angers, SFR MATRIX, Angers, France; [6] National Institute for Laser, Plasma and Radiation Physics, Bucharest-Magurele, Romania

The integration of two or more different lanthanide ions in a single compound can generate molecular materials with applications in magnetism[1], spintronics[2], or upconversion luminescence[3], attributed to the remarkable magnetic and luminescent properties that emerge from the electronic configuration of the 4*f* metal ions. Although it appears straightforward, the main challenge lies in the preparation of pure heterometallic 4*f*-4*f'* complexes, since statistical mixtures might occur due to the similar chemical properties of the lanthanide ions. To address this limitation, a synthethic strategy has been adopted in this work that emphasizes the design of asymmetric compartmental ligands capable of selectively acommodating two different lanthanides ions according to their ionic radii.
Hence, a novel family of octanuclear complexes, $[Ln_4Yb_4]$, is synthesized using a Schiff base ligand ($\mathbf{H_4L^1}$) obtained from the condensation of 2-hydroxy-3-(hydroxymethyl)-5-methylbenzaldehyde with 1,8-diamino-3,6-dioxaoctane: $[Ln_4Yb_4(\mathbf{L^1})_2(\mathbf{HL^1})_2(NO_3)_8(X)(Y)(\mu_4\text{-}O)]$, where Ln = Nd (**1**), Sm (**2**), Eu (**3**), and X=Y= MeOH and/or H_2O. The employment of another Schiff base ligand ($\mathbf{H_4L^2}$), which is derived from 2,3-dihydroxybenzaldehyde and 1,8-diamino-3,6-dioxaoctane, leads to the generation of the following complexes: $[Ln_{(4\text{-}x)}Yb_4\mathbf{L}_{(4\text{-}x)}(\mathbf{H_2L^2})_x(NO_3)_4(CH_3COO)_{(4\text{-}x)}(\mu\text{-}H_2O)]$, where Ln = Pr(**4**), Nd(**5**) and x = 0.72 (**4**), 0.56 (**5**). All compounds have been characterized by single crystal X-ray diffraction, mass spectrometry, UV-VIS and IR spectroscopy. The photoluminescent properties of complexes **1-3** have been evaluated.

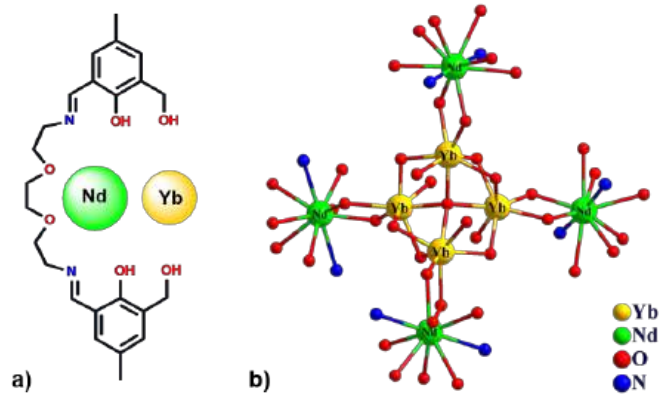

Fig 1. a) Schematic representation of the $\mathbf{H_4L^1}$; b) View of the central cluster core of **2**

Acknowledgements: This work was supported by a grant of the Ministry of Education and Research, CCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053 (Contract no. 5CoEx/2026; ChemBioCatCirEcon) within PNCDI IV.

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MDR - D2 – P11
Functionalized hydrosilanes: Pathways to silicon-based semiconductors

Daniel Griess[1], Michael Haas[1,*]
Institute of Inorganic chemistry, Graz University of Technology, Austria
**Email: griess@tugraz.at*

Conventional semiconductor manufacturing based on single-crystal silicon wafers is cost-intensive due to high energy requirements and substantial material waste, with only about 25% of the single-crystal silicon ultimately utilized.[1] Hydrosilanes (HS) offer a viable alternative, mitigating both energy and waste challenges while serving as promising starting materials for the liquid-phase deposition (LPD) of high-quality silicon layers.[2,3] Functionalized hydrosilanes (FHS) expands their utility for semiconductor fabrication by addressing the current lack of synthetic pathways that deliver both high silicon content and precisely controlled heteroatom doping levels.[4] In this lecture, we present recent advances in FHS chemistry and materials manufacturing. Figure 1 summarizes the general strategy of the LPD process for carbon-functionalized hydrosilanes.[5]

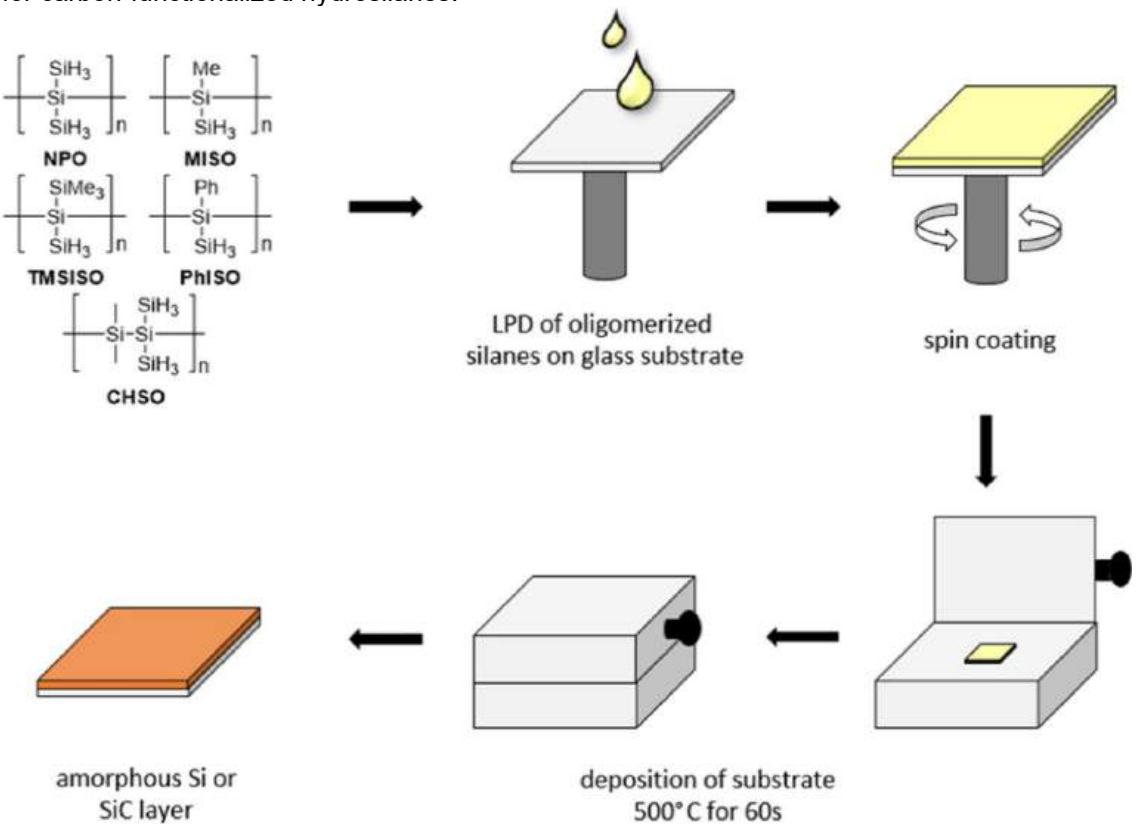

Fig. 4. General procedure of the LPD process of oligomeric mixtures.[5]

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MDR - D2 – P12
Lanthanide and transition metal complexes derived from polydentate Schiff bases

Robert I. Botea, Augustin Mădălan
Faculty of Chemistry, University of Bucharest, Romania

Polydentate Schiff base ligands derived from N-(1-naphthyl)ethylenediamine and substituted salicylaldehydes were employed for the synthesis of mono- and heteronuclear coordination complexes with 3d, 4d, and 4f metal ions. Owing to their extended π-conjugated systems and multiple coordination sites, these ligands enable the formation of structurally and functionally diverse metal complexes with enhanced stability and tunable physicochemical properties.
Mononuclear complexes of Zn(II), Cu(II), Pd(II), Eu(III) and Tb(III) were synthesized by reacting the Schiff base ligands with appropriate metal salts and were fully characterized using spectroscopic techniques and single-crystal X-ray diffraction. The solid-state structures revealed various coordination geometries: tetrahedral, square-planar, square pyramidal and octahedral for the transition metal complexes, respectively square-antiprismatic environments for the lanthanide derivatives. A representative synthetic route for the 3d metal complexes is shown in Figure 1.

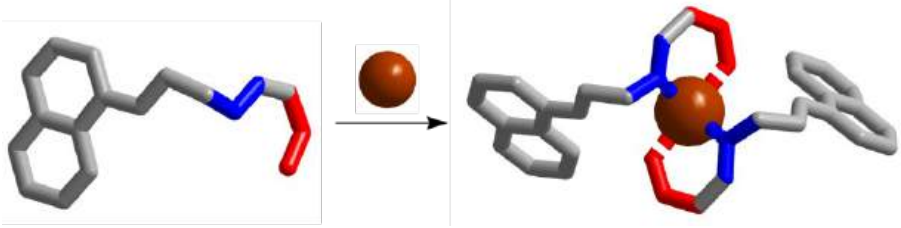

Fig. 5. Schematic synthesis of 3d complexes using Schiff base ligands.

Luminescence studies demonstrated characteristic emissions for the Eu(III) and Tb(III) complexes, originating from efficient ligand-to-metal energy transfer processes facilitated by the π-extended ligand framework. Furthermore, stepwise synthetic strategies enabled the formation of heterometallic Zn-Ln complexes, in which the initial coordination of Zn(II) provides preorganization of two imino ligands for subsequent lanthanide incorporation. These heteronuclear systems exhibit enhanced luminescent properties compared to the corresponding mononuclear analogues.
Particular attention was devoted to Pd(II) complexes due to their potential interactions with biomolecules (nucleic acids). Their square-planar geometry and the pendant aromatic fragments of the ligands make these compounds promising candidates for further investigation as intercalating agents. Figure 2 presents the X-ray crystal structures of two Pd(II) complexes with different metal-to-ligand stoichiometries.

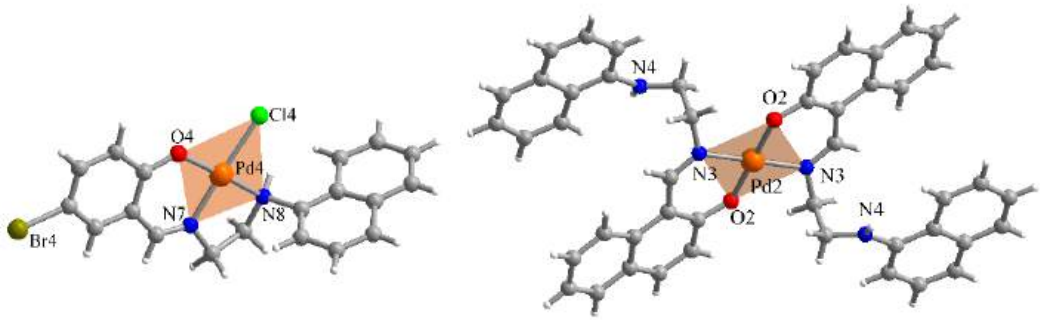

Fig. 6. X-ray crystal structures of two Pd(II) complexes featuring 1:1 and 1:2 metal-to-ligand ratios.

MDR - D2 – P13

Design of optically-active coordination compounds using various ligands showing different types of chirality

Valentin L. Virgil[1,2], Simona Nica[2], Cătălin Maxim[1], Marius Andruh[1,2]
[1]University of Bucharest, Faculty of Chemistry, Romania; [2]"Costin D. Nenițescu" Institute of Organic and Supramolecular Chemistry, Romania

The chiroptical properties of Ln(III) coordination systems arises from the intrinsic nature of their electronic transitions, where the parity-forbidden 4f-4f transitions often exhibit significant magnetic dipole-allowed character. In the framework of the Rosenfeld equation, the magnitude of g_{lum} is proportional to the ratio between the magnetic dipole transition moment and the electric dipole transition moment.[1] Furthermore, the structural modularity of coordination chemistry allows for the precise transmission of chiral information within the coordination spheres.This geometric control, combined with the narrow emission bandwidths and long-lived excited states characteristic of lanthanides, make these type of complexes potential candidates for optoelectronic devices.[2]
Our research focuses on synthesizing optically active 3d–4f complexes using enantiopure Schiff-base ligands derived from *o*-vanillin and chiral diamines. By employing diamagnetic Zn(II) ions to preserve the 4f-centered luminescence, we aim to facilitate the transfer of chiral information from the ligand to the Ln(III) ion to induce circularly polarized luminescence. Our preliminary results consist of a Zn(II)–Tb(III) enantiomeric pair in which the Tb(III) ion shows CPL activity (Figure 1).

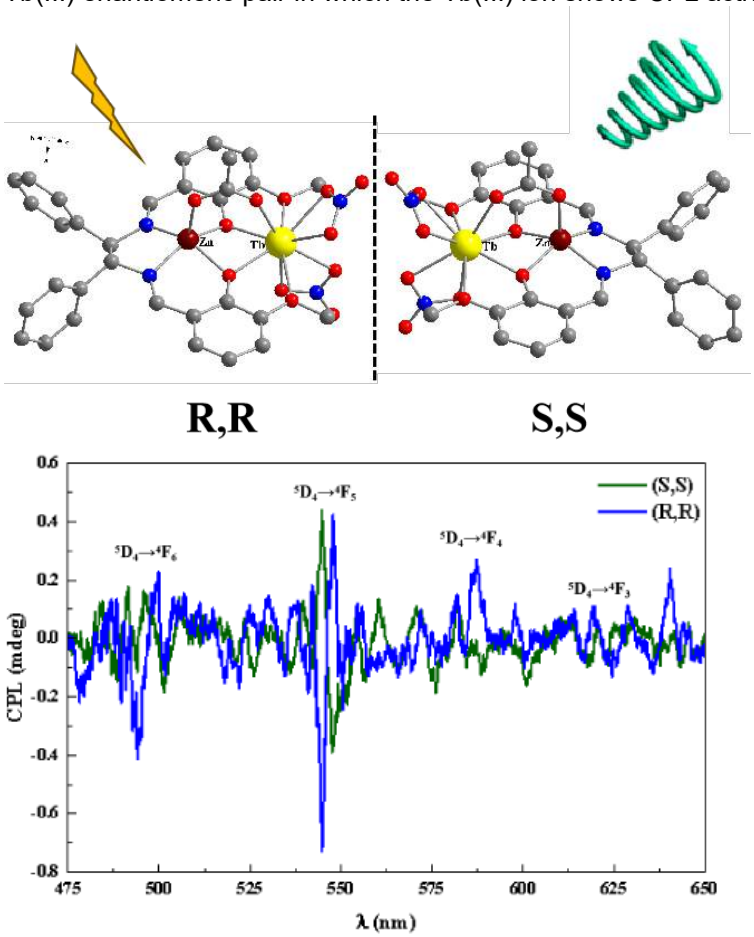

Fig 1. The molecular structure and the CPL spectra of the enantiomeric pair (R,R)-[ZnTb(L)(ac)$(NO_3)_2$] and (S,S)-[ZnTb(L)(ac)$(NO_3)_2$].

Acknowledgements: This work was supported by a grant of the Ministry of Education and Research, CCCDI-UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV.

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MDR - D2 – P14

Redirecting a synthetic dead-end to an antimalarial compound with enhanced activity

Daniela Silva dos Santos[1], Benedikt Kolb[1], Fabian Schmid[1], Jessica Weng[1], Luca Altevogt[1], Ruben Pereira Rebelo[1], Bianca Wank[1], Angelika Baro[1], Anna Zens[1], Aditya Shekhar[2], Ursula Bilitewski[2], Sibylle Sax[5], Sergio Wittlin[5], Dale Taylor[4], Rudolf Müller[3], Sabine Laschat[1]
[1]Institut für Organische Chemie, Universität Stuttgart,Germany; [2]AG Compound Profiling and Screening, Helmholtz Zentrum für Infektionsforschung, Germany; [3]Drug Discovery and Development Centre (H3D), Dept. of Chemistry, University of Cape Town, South Africa; [4]Drug Discovery and Development Centre (H3D), Division of Clinical Pharmacology, Dept. of Medicine, University of Cape Town, South Africa; [5]Parasite Chemotherapy, Swiss Tropical and Public Health Institute, University of Basel, Switzerland

Malaria remains a disease of high medical relevance, and with rising incidence of drug resistance, we pursued the development of a novel synthetic strategy of samroiyotomycin A. This natural product is highly active against malaria but suffers from limited synthetic accessibility. Therefore, we synthesized the enantiopure *syn-syn*-tosyl-samroiyotomycin A in 7 linear steps and an overall yield of 3 %, employing a sequence of [Rh]-catalyzed cross-metathesis to assemble the *seco*-acids from the acids and alcohols, followed by esterification/macrolactonization. Attempts to cleave the tosyl-group to isolate the *syn-syn*-samroiyotomycin A remained unsuccessful. In addition, the corresponding diastereomer and a series of related macrodiolides carrying phenyl, benzyl or other heteroaryl unit instead of oxazole were synthesized.
Detailed biological profiling was performed against Plas*modium falciparum*, including both chloroquine-sensitive (NF54) and multi-drug resistant (K1) strains, for the *syn-syn*-tosyl-samroiyotomycin A and the "tosyl-free" natural product. Biological investigations revealed a remarkable antiplasmodial activity of *syn-syn*-tosyl-samroiyotomycin A, which is 3.4 x times more active than the "tosyl-free" natural product, indicating that the targeted structural modification can enhance biological properties.
Due to the limited biological information and with the aim of elucidating structure-activity relationships, we further profiled samroiyotomycin A, its derivatives, and synthetic key precursors. The results revealed the crucial role of the tosyl-protecting group, both in the synthetic strategy and biological activity. Additionally, these studies provide initial insights into the pharmacophoric subunits of *syn-syn*-samroiyotomycin A that are critical to its antiplasmodial properties.
This work not only demonstrates a practicable synthetic route to a structurally intricate antimalarial macrodiolide but also highlights how synthetic analogues can improve upon natural lead structures.

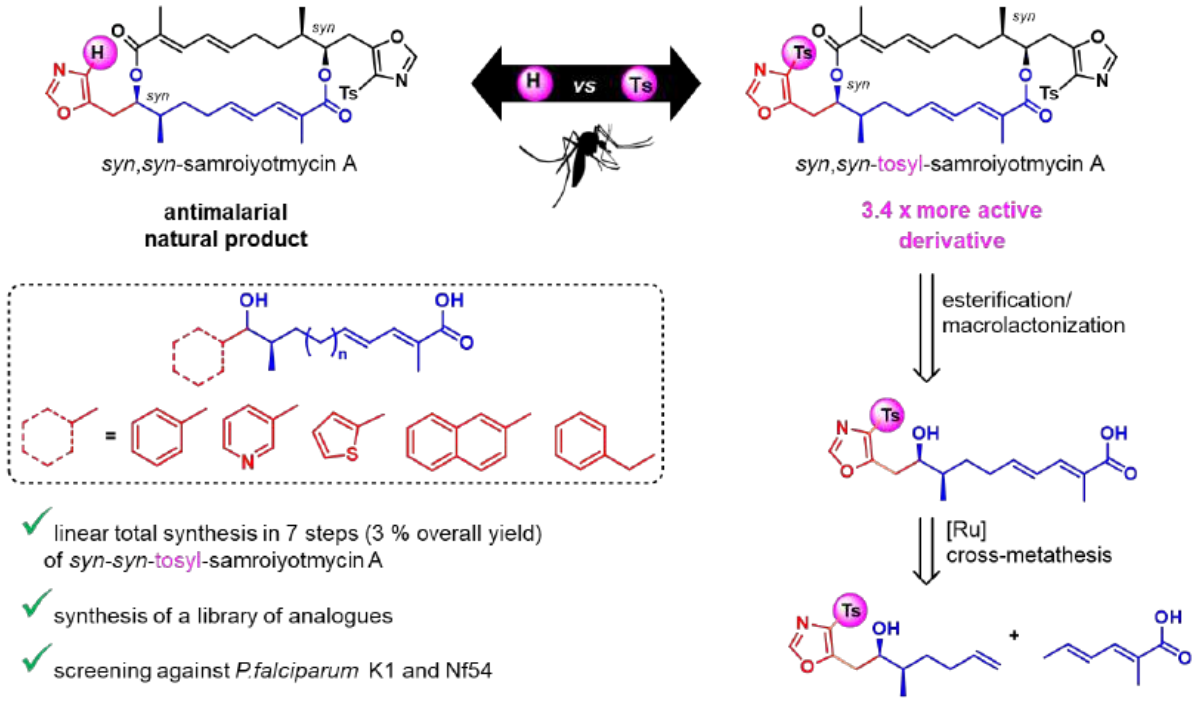

Fig 1. Retrosynthetic analysis of *syn*-*syn*-tosyl-samroiyotomycin A *via* cross-metathesis and esterification/macrolactonization. Substrate library of derivatives with different substituents instead of the oxazole ring.

Funding was provided by the Deutsche Forschungsgemeinschaft (HBFG and shared instrumentation grant no. INST 41/897-1 FUGG for 700 MHz-NMR), the Ministerium für Wissenschaft, Forschung und Kunst des Landes Baden-Württemberg and Fonds der Chemischen Industrie.

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MDR - D2 – P15

Design of hetero-functionalized triarylamine-based scaffolds as open-shell electrophoto-catalysts

Lukas Dvorak[1], Oda Fossheim[1], Audun Formo Buene[1]
[1]Dept. of Chemistry, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Electrophotocatalysis (EPC) is a powerful tool in organic synthesis that combines photoredox catalysis and electrosynthesis to access highly reactive redox states under mild and well-controlled conditions. While photoredox catalysis is limited by the energy of absorbed photons and electrosynthesis by the electrochemical window of the solvent, their combination enables a broader effective redox window for single-electron transfer processes and reduces the need for harsh or stoichiometric reagents.[1,2]
This work focuses on the design of hetero-functionalized triarylamine-based scaffolds as organic open-shell electrophotocatalysts for oxidative transformations. Building on established triarylamine systems, hetero-functionalized T*p*BPA derivatives are explored in which electronically distinct substituents on individual aryl units create push–pull electronic effects, enabling tuning of redox properties and radical cation stability. Unsymmetrical substitution patterns may further promote preferential substrate orientation, potentially leading to enhanced chemo- or regioselectivity.
The synthesized catalysts are evaluated in representative electrophotocatalytic reactions, supported by electrochemical and photophysical characterization to establish structure–property relationships. Overall, this work aims to expand the scope of organic electrophotocatalysis through rational catalyst design.

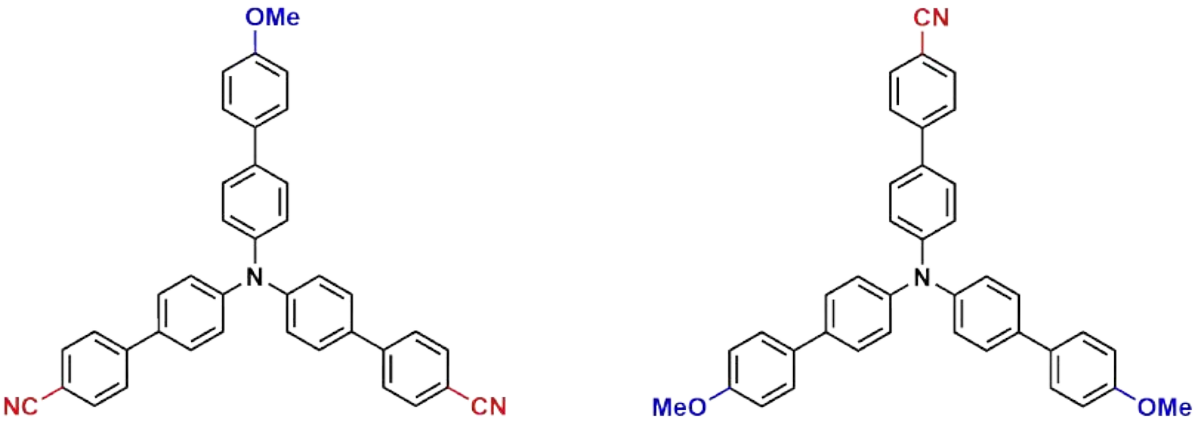

Fig 1. Representative hetero-functionalized triarylamine-based scaffolds used as open-shell electrophotocatalysts.

The authors acknowledge support from the Anders Jahres Fund for the Advancement of Science for funding equipment used to establish the electrophotocatalysis setup.

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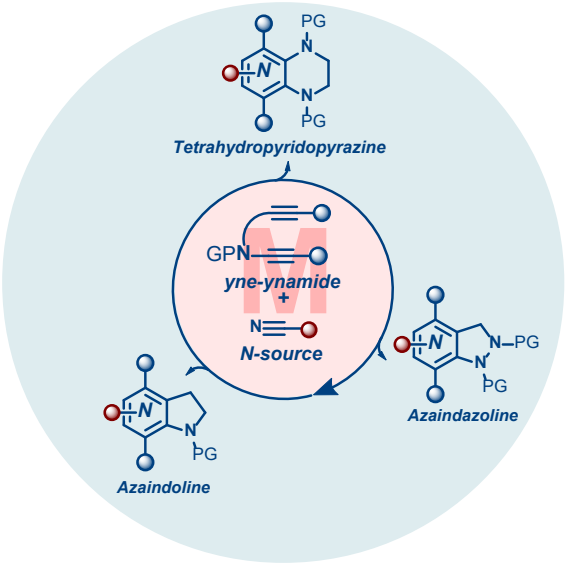
MDR - D2 – P16
Metal-catalysed assembly of *N*-heterocycles via [2+2+2] cyclisation

Ana A. Reis[1], Edward A. Anderson[2], Maria Manuel B. Marques[1]
[1]LAQV-REQUIMTE, NOVA FCT, Portugal; [2]Chemistry Research Laboratory, University of Oxford, UK

N-Heterocycles are fundamental structural motifs in medicinal chemistry and are found in most FDA-approved small-molecule drugs[1]. Consequently, there is a strong demand for new synthetic strategies to access these scaffolds with a high degree of functionalisation. Metal-catalysed [2+2+2] cycloaddition (cyclotrimerisation) of yne-ynamides has emerged as an atom-economical and efficient method for constructing highly functionalised *N*-heterocycles[2-5]. Herein, we report a metal-catalysed cyclotrimerisation between yne-ynamides and *N*-sources that provides a diverse range of highly functionalised heterocyclic scaffolds (**Scheme 1**).



Scheme 1. Metal-catalysed cyclotrimerisation of alkyne-ynamides with *N*-sources, affording a diverse array of highly functionalised *N*-heterocycles.

Acknowledgments: The authors thank FCT for projects PTDC/QUI-QOR/0712/2020 and fellowship reference 2023.00810.BD and DOI identifier https://doi.org/10.54499/2023.00810.BD. "This work was funded by national funds from FCT - Fundação para a Ciência e a Tecnologia, I.P., under the scope of the projects UID/50006/2025, UID/PRR/50006/2025 and LA/P/0008/2020 of the Associated Laboratory for Green Chemistry - LAQV REQUIMTE (https://doi.org/10.54499/UID/50006/2025, https://doi.org/10.54499/UID/PRR/50006/2025 and https://doi.org/10.54499/LA/P/0008/2020)." The National NMR Facility is supported by FCT,ROTEIRO/0031/2013–PINFRA/22161/2016, co-financed by FEDER through COMPETE 2020, POCI, and PORL and FCT through PID-DAC) and CERMAX (022162). E.A.A. thanks the EPSRC for additional support (EP/S013172/1).

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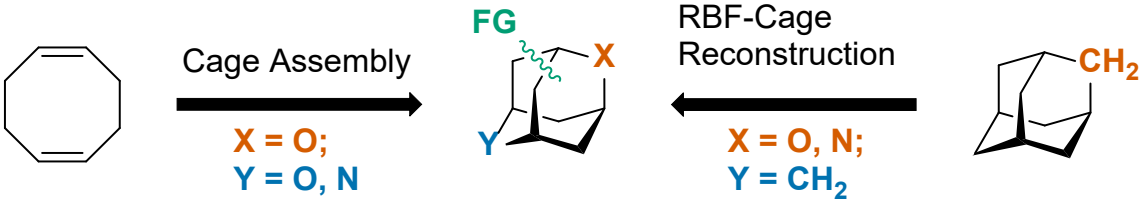
MDR - D2 – P17

Preparative-scale synthesis of heteroatom-doped adamantanes and their MedChem evaluation

Ioann Popov[1,2,3], Dmytro Volochnyuk[1,2,3,4], Olexandr Pashenko[2,4], Serhiy Ryabukhin[1,2,3,4]
[1]Enamine Ltd, Ukraine; [2]Taras Shevchenko National University of Kyiv, Ukraine; [3]Institute of Organic Chemistry, NAS of Ukraine; [4]Enamine Scientific Research Institute, Ukraine

Adamantane scaffolds are found in multiple approved pharmaceuticals with antiviral (amantadine, rimantadine), neuroprotective (memantine), and enzyme-inhibitory (saxagliptin, vildagliptin) activity. Their rigidity, high sp^3 character, and metabolic stability make them privileged structures in medicinal chemistry. However, all-carbon adamantanes often exhibit suboptimal ADMET profiles, particularly excessive lipophilicity and poor aqueous solubility, which restrict their therapeutic applications. Heteroatom-doped adamantanes incorporating oxygen and secondary nitrogen atoms represent rational bioisosteric replacements expected to address these liabilities by enhancing polarity and hydrogen-bonding capacity, while preserving the beneficial three-dimensional cage topology and conformational rigidity. Despite a convincing rationale, systematic pharmaceutical investigation has been impossible due to a fundamental synthetic bottleneck: traditional routes require complex, multi-step cage-fragmentation-reconstruction sequences that often employ hazardous reagents, resulting in low efficiency and limiting preparative-scale access. We report comprehensive optimization of retro-Barbier fragmentation (RBF)-reconstruction[1] and cyclooctadiene-derived cage assembly[2] methodologies, specifically targeting 2-oxa-, 2-aza-, 2,6-dioxa-, and 2-oxa-6-aza-adamantane cores, as well as related cage structures. Our refined protocols eliminate the need for hazardous reagents, streamline synthetic sequences, and achieve good to excellent isolated yields, with confirmed, reproducible throughput reaching tens to hundreds of grams per operation. This preparative-scale capability provides sufficient material for extensive C–H functionalization studies, as well as downstream derivatization campaigns, and creates an opportunity for systematic structure-activity relationship exploration previously precluded by material scarcity. Our optimized routes transform heteroadamantanes from synthetically inaccessible targets into practical pharmaceutical scaffolds, enabling ongoing comprehensive ADMET evaluation, reactivity profiling, and assessment as advanced adamantane replacement cores where improved physicochemical properties are therapeutically critical.



Cage assembly and RBF-reconstruction-based approaches to bis- and mono-heteroadamantanes.

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MDR - D2 – P18

End-group positioning enables selective demicellization in self-immolative poly(benzyl ether) micelles

Hyungwoo Kim
School of Polymer Science and Engineering, Chonnam National University, Gwangju, Korea

This presentation introduces the molecular design of degradable micelles constructed from self-immolative poly(benzyl ether)-based amphiphilic block copolymers. These micelles undergo stimulus-triggered demicellization through a head-to-tail depolymerization mechanism, which is initiated by the cleavage of a terminal end group. The amphiphilic copolymers were synthesized via living anionic polymerization by sequential addition of two quinone methide monomers, enabling precise control over block sequence and end-group placement. In the first micelle system, the reactive end groups are embedded within the hydrophobic core, resulting in high structural stability in aqueous media (Figure 1, top). These micelles effectively encapsulate hydrophobic cargo and suppress premature release. Upon exposure to a specific stimulus, the trigger diffuses into the micelle core and activates depolymerization from the end group, leading to controlled cargo release. However, because the end group is spatially confined within the core, the demicellization rate is limited, which may restrict applications requiring rapid disassembly. To enhance depolymerization efficiency, we modified the polymerization sequence to reposition the reactive end group toward the micelle corona/exterior (Figure 1, bottom). This design enables immediate access to external stimuli, thereby accelerating depolymerization and promoting faster, more uniform demicellization. Overall, this end-group relocation strategy provides a practical route to achieving selective and programmable micelle disassembly for responsive delivery systems.

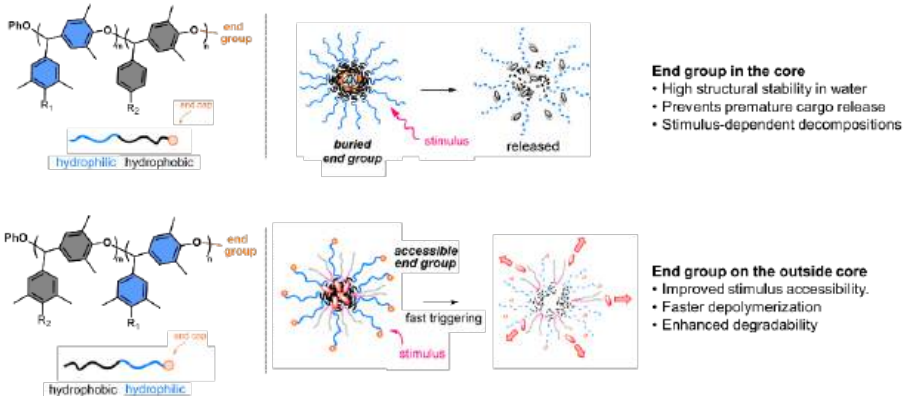


Fig 1. Molecular strategies for demicellization of self-immolative poly(benzyl ether) amphiphiles: (top) core-to-surface depolymerization and (bottom) surface-to-core depolymerization.

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (RS-2025-25404226).

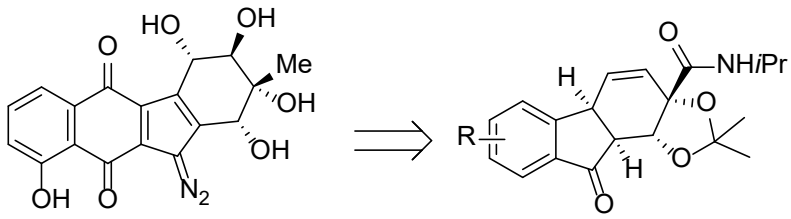
MDR - D2 – P19

Studies towards applying a palladium-catalysed arylation-acylation domino reaction for a new total synthesis of kinamycin F

Mees M. Hendrikx[1], Agnes Ingvarsson[1], Lorenzo Celio[2], Petter Dunås[1], Andrew J. Paterson[1], Simon E. Lewis[3], Nina Kann[1]

[1]Dept. of Chemistry and Chemical Engineering, Chalmers University of Technology, Sweden; [2]Dept. of Chemistry, Sapienza University of Rome, Italy; [3]Centre for Sustainable Circular Technologies & Dept. of Chemistry, University of Bath, UK

Domino reactions are chemical reactions where two reactions occur consecutively, where the second reaction follows from the formation of a functional group in the first reaction, allowing the rapid creation of molecular complexity. The serendipitous discovery of a domino reaction, where a Heck-type reaction proceeds a ring closing acylation to form a 9-fluoreneone core,[1] opens a potential new pathway to a total synthesis of the benzo[*b*]fluorene-containing natural product kinamycin F. Kinamycins are a family of natural products found in several species of bacteria, of interest due to their antibiotic and anticancer activities through a novel mechanism.[2] This work details the preliminary results of an investigation into an alternative total synthesis of kinamycin F with a palladium-catalysed arylation-acylation domino reaction as the pivotal step.[1] Utilizing a whole-cell biocatalysed dearomatisation-dihydroxylation of benzaldehyde by *Cupriavidus necator* B9 the carbon scaffold of the right-hand part of the kinamycin skeleton can be produced. The first steps for obtaining the starting material for the left-hand part of kinamycin are presented here, including modifications and alternative routes. Further reactions are proposed to guide future work.



Kinamycin F

Scheme 1. Retrosynthesis for kinamycin F from the domino reaction product.

The Swedish Research Council is gratefully acknowledged for funding (grant nr. 2023-0434).

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MDR - D2 – P20

Nitronyl nitroxide di- and triradical ligands obtained *via* Schiff condensation and their complexes

Mihai Răducă[1,2], Iulia-Cristiana Muscalu[1], Sergiu Shova[3], Gabriela Ioniță[4], Floriana Tuna[5], Marius Andruh[1,2]

[1]Faculty of Chemistry, University of Bucharest, Romania; [2]Costin D. Nenițescu Institute of Organic and Supramolecular Chemistry of the Romanian Academy, Romania; [3]Petru Poni Institute of Macromolecular Chemistry, Romania; *[4]Ilie Murgulescu Institute of Physical Chemistry of the Romanian Academy, Romania; [5]Dept. of Chemistry and Photon Science Institute, University of Manchester, UK*

The design of ligands incorporating nitronyl nitroxide (NN) unit(s) generally follows two principal synthetic strategies. In the first approach, aldehyde functionalities present in the molecular scaffold are converted into the corresponding NN radicals, thereby directly generating the target ligand [1]. In the second approach, a preformed NN radical is covalently attached to a substrate *via* suitable reactions such as cross-coupling [2], alkylation [3] or, as in the present case, Schiff condensation [4]. The NN bearing free formyl unit, HL^1, has been used to form di- and triradical ligands with various amines: notably 4-amino-TEMPO (HL^2) and tris(2-aminoethyl)amine (H_3L^3) (Figure 1). The paramagnetic ligands have been reacted with hexafluoroacetylacetonate ($hfac^-$) complexes ($[M(hfac)_2(H_2O)_2]$ and $[Ln(hfac)_3(H_2O)_2]$ where M = Co, Ni, Zn and Ln = Gd, Tb, Dy) yielding mono-, di- and trinuclear complexes with various topologies. The structures have been analyzed using X-ray diffraction on single crystal both for the ligands and the complexes and the EPR spectra have been recorded for the di- and triradical species indicating exchange interactions between radical moieties.

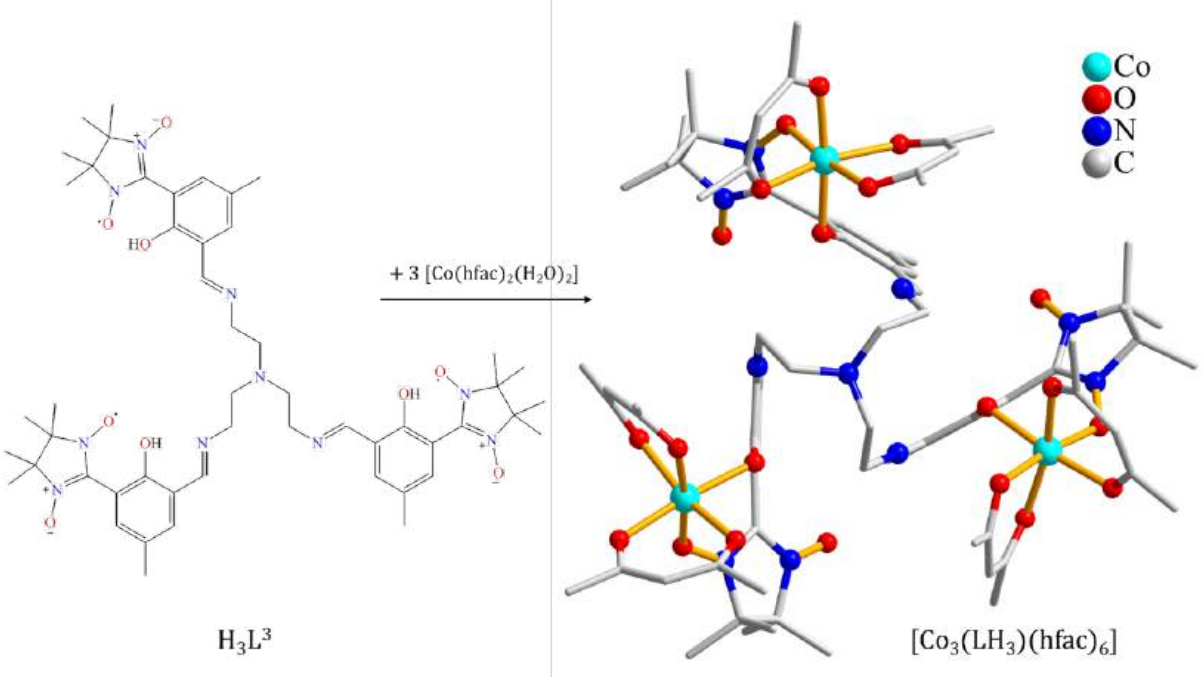

Fig. 7. The crystal structure of the trinuclear complex $[Co_3(LH_3)(hfac)_6]$ obtained from tripodal triradical ligand H_3L^3. Hydrogen and fluorine atoms have been omitted for clarity.

This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV and from European Union through the NextGeneration EU-PNRR−III-C9-2022-I8 program (contract no. 760230).

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MDR - D2 – P21

Synthesis and magnetic properties of a family of dinuclear lanthanide complexes derived from 2-(phthalimidomethyl)-nitronyl-nitroxide

Ștefan Dimitriu[1,2], Mihai Răducă[1,2], Diana-Ioana Eftemie[1,2], Marius Andruh[1,2]
[1]University of Bucharest, Faculty of Chemistry, Romania; [2]"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry, of the Romanian Academy, Romania

Nitronyl-nitroxides (NITs) have a rich coordination chemistry, allowing the synthesis of complexes with various spin topologies that show intriguing magnetic properties. While the vast majority of NITs reported in the literature are obtained starting from the corresponding aldehydes,[1] methods of grafting the radical unit onto a substrate through coupling or alkylation[2] reactions have also been described, benefiting from simpler procedures and higher yields. This work focuses on a new paramagnetic ligand obtained through the alkylation of phthalimide with 2-(chloromethyl)-nitronyl-nitroxide.[1] The study of its coordination chemistry afforded two structural families of complexes (Figure 1). Their structures were solved by single-crystal X-ray diffraction measurements. The complexes with transition metal ions (Ni^{II}, Co^{II}) are mononuclear species and display two ligand molecules bound to the metal ion through the radical moiety. The complexes with lanthanides (Pr^{III}, Nd^{III}, Eu^{III}, Gd^{III}) are dinuclear, having both metal ions coordinated by the radical moiety. Consequently, two systems, with 2p-3d-2p and 4f-2p-4f spin topologies, have been obtained. The magnetic properties of the lanthanide complexes family have been investigated. In the case of the gadolinium complex, the temperature dependence of $\chi_M T$ reveals a ferromagnetic interaction for the Gd-NIT-Gd system, The fitting of the experimental data yielded significantly different Gd-NIT coupling constants (6.8 and 0.2 cm^{-1}, $\boldsymbol{H}=-J_1\boldsymbol{S}_{Gd1}\boldsymbol{S}_{NIT}-J_2\boldsymbol{S}_{NIT}\boldsymbol{S}_{Gd2}$), which can be explained by the difference in the geometrical parameters observed in the crystal structure.

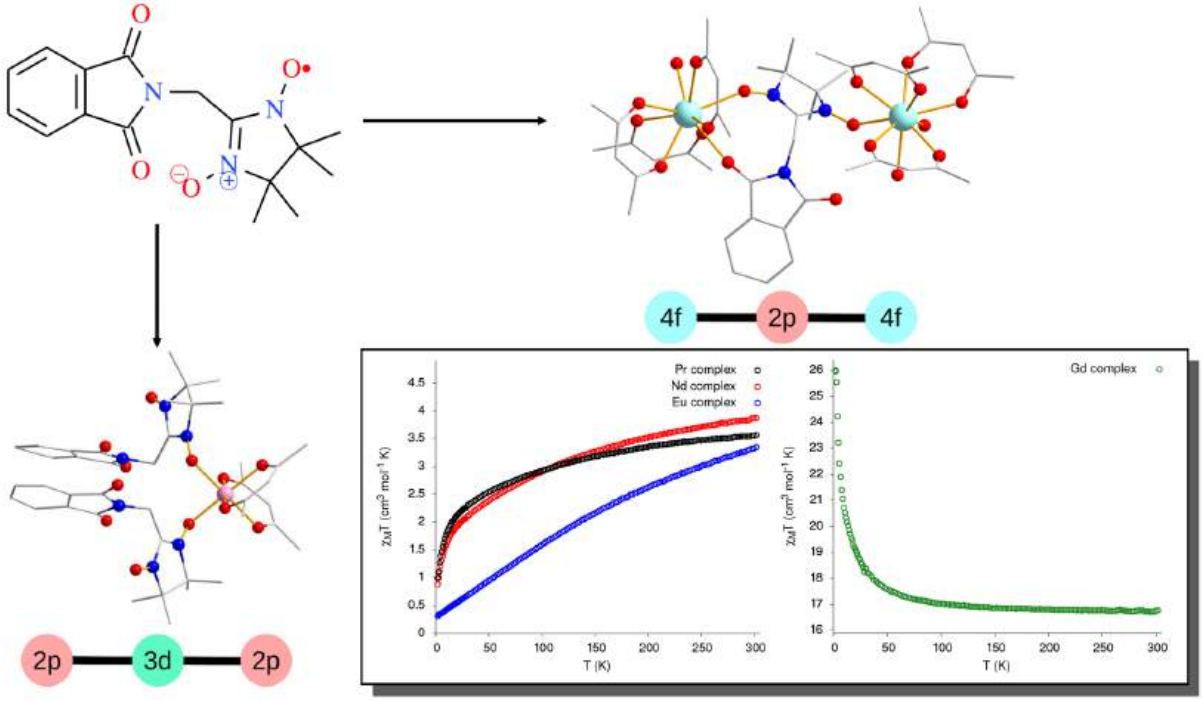

Fig 1. The structure of 2-(phthalimidomethyl)-nitronyl-nitroxide, its complexes with transition metals and lanthanide ions, and the $\chi_M T$ versus T plots recorded for the lanthanide complexes.

This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV.

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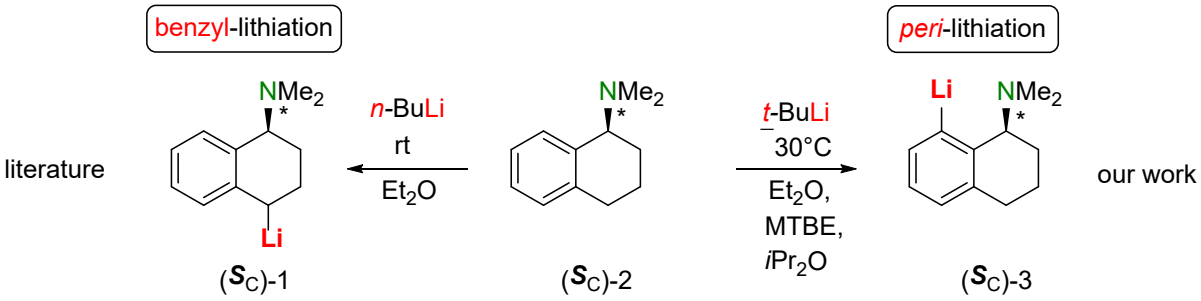
MDR - D2 – P22

Peri- and benzyl-lithiation of a chiral bicyclic amine: Solvent-controlled regioselectivity

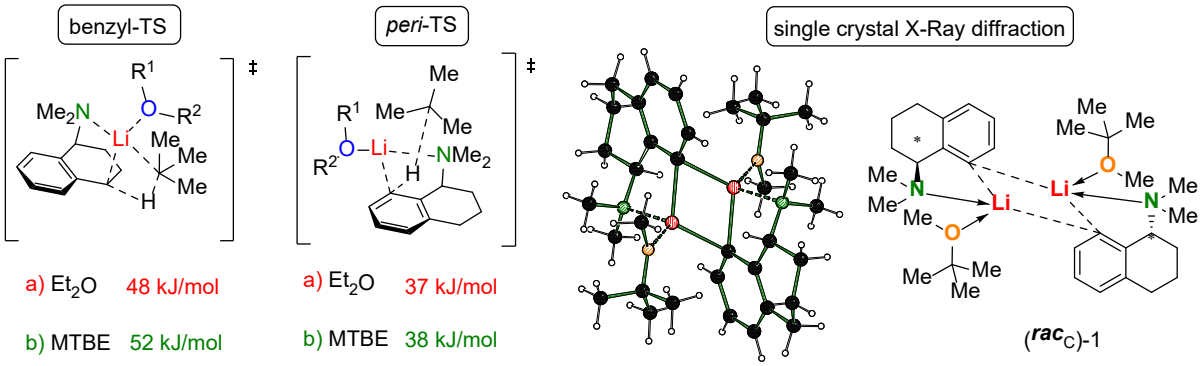
Franziska Dorothea Klotz[1], Anna Krupp[1], Carsten Strohmann[1]
[1]*Faculty of Chemistry and Chemical Biology, TU Dortmund University, Germany*

Directed lithiation is among the most powerful tools for the regioselective functionalization of aromatic frameworks. However, substrates capable of undergoing deprotonation at more than one position frequently exhibit competing pathways, with regioselectivity often governed by subtle combinations of electronic, steric, and solvation effects.[1]



Scheme 1. Lithiation reaction of 5,6,7,8-tetrahydro-1-naphthylamine with different etheric solvents.

In case of the bicyclic amine 5,6,7,8-tetrahydro-1-naphthylamin investigated in our work, two deprotonation sites, the benzyl- and the *peri*-position, are accessible. Early studies by *Saegusa et al.* reported the formation of both regioisomers in a 33:67 ratio (*peri*:benzyl).[2] By using *t*-BuLi as a base we were able to reverse the selectivity towards the *peri*-lithiated substrate to 75:25. Changing the reaction conditions to low temperatures and by systematically varying the steric demand of etheric solvents, regioisomer-ratios up to 98:2 were obtained.



Scheme 2. Quantum chemical calculations [M062x, 6-311 G(*d,p*)] on the transition state of the lithiation and single crystal analysis of the lithiated product.
Using MTBE, diethyl ether and diisopropyl ether, we demonstrate that the steric bulk and donor ability of the ether ligand determine the coordination environment of the lithium cation and thereby govern the deprotonation pathway. Moreover, quantum-chemical calculations allowed us to compare the transition states in different solvents, providing a mechanistic explanation for the observed regioselectivities. We successfully obtained single crystals of the lithiated intermediates crystallized from MTBE and Et_2O and confirmed their structure in solution by DOSY-NMR experiments.

A scholarship from the *Studienstiftung des deutschen Volkes* was awarded to F. D. K.

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MDR - D2 – P27

A single component chemical system to encode complex temporal evolution of pH

Daniele Del Giudice[1], Giorgio Fusi[2], Alessandro Nardi[3], Roy Wink[1], David Attia,[1] Esmee De Korver,[1] Bert Meijer[1]

[1]Institute for Complex Molecular Systems and Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, The Netherlands; [2] Dept. of Chemistry, University of Mainz, Mainz, Germany; [3]Nantes Université, CNRS, CEISAM, UMR 6230, Nantes, France

The achievement of artificial systems capable of being maintained in out-of-equilibrium states featuring functional properties is a main goal of current chemical research.[1] Absorption of electromagnetic radiation or consumption of a chemical species are the two strategies typically employed to reach such dissipative states, which persist as long as one of the above stimuli is present. Many of the dissipative artificial systems reported so far are driven by bioinspired reactants such as nucleoside triphosphates (ATP, GTP) or fragments of RNA/DNA, and often take advantage of the presence of enzymes for their operation.[2] Recently, several fully abiotic dissipative systems have been developed, such as activated carboxylic acids (tribromoacetic acid, TBA, and trichloroacetic acid, TCA).[3] These have been widely used to control the operation of a variety of pH-responsive systems and devices, by exploiting the transient pH variation resulting from their base-catalyzed decarboxylation. However, the operation mechanism of such systems is generally simpler, and does not allow to obtain the same degree of complexity achievable with enzymes. Here, we employed esters of activated carboxylic acids, namely ethyl tribromo- and trichloroacetate (ETBA and ETCA respectively), disclosing a new level of control over aqueous solution pH by means of a single chemical reactant. This approach enables the generation of an initial lag time, followed by a transient state, both of which can be finely tuned in time. As a proof of concept, we applied this strategy to perylene diimide (PDI) based supramolecular polymers, achieving precise control on their selfassembly both in space and time.

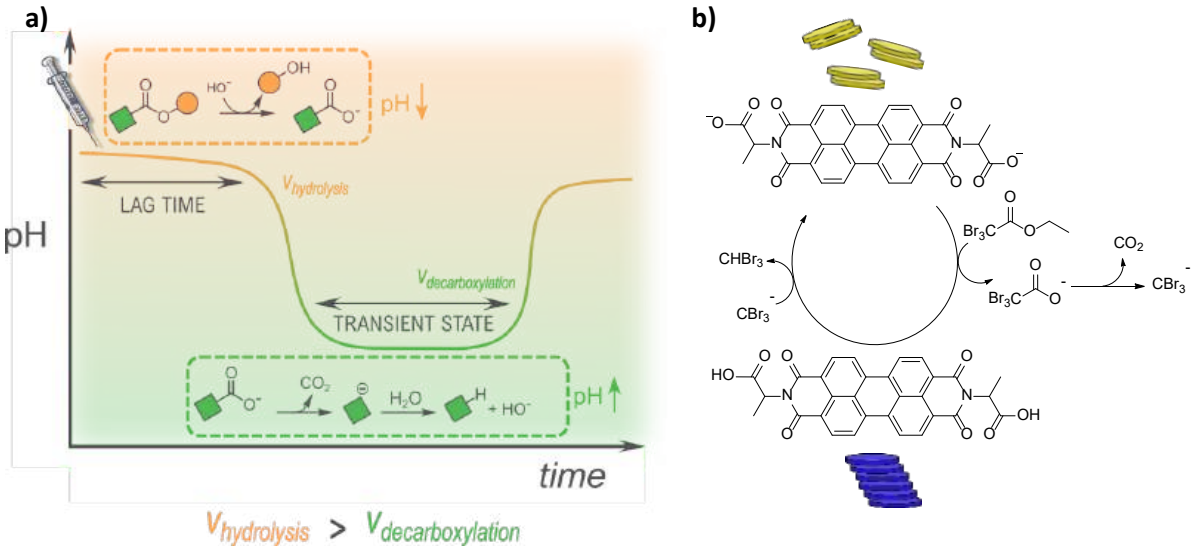

Fig 1. a) Chemical reaction network triggered by esters of activated carboxylic acids. b) Transient selfassembly of PDI-based supramolecular polymers under the effect of ethyltribromoacetate.

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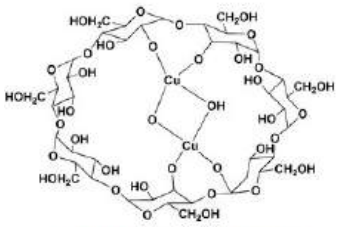
MDR - D2 – P28

Exploratory studies on the mechanosynthesis of the copper(II) β -cyclodextrin complex

Amanda Beatriz S. Q. dos Reis[1], Marcos Vinícius M. Ribeiro[1], Alexsandro A. Silva[1], Stéphane Menuel[2], Eric Monflier[2], Anne Ponchel[2], Luiz Fernando B. Malta[3], Jaqueline D. Senra[1]
[1]UERJ, Brazil; [2] Universitè d'Artois, France; [3]UFRJ, Brazil

The coordination of Cu(II) ions by β-CD, in alkaline solution, was firstly reported by Messmer[1] in 1927. Since then, several works have reported the performance of this uncommon complex as catalyst in a number of organic reactions[2]. In this case, a binuclear structure with bridged Cu-O bonds are proposed through the secondary hydroxyl groups[1]. However, the synthesis route presents some inconvenience such as strongly basic medium and a relatively long reaction time. As a result, the complex is generally obtained in low yields due to the formation of copper oxides as by-products. To the best of our knowledge, there is no report on the modified synthesis of this complex. Herein, we propose a mechanochemical approach via dry-milling for its synthesis using a vibratory ball-milling with $CuSO_4.H_2O$, □-CD and KOH as reagents in a 2:1:3 stoichiometry, with 20 Hz during 1 - 2h. Control experiments were also carried out in solution. The material was characterized by DRS, Raman spectroscopy and XRD. The UV-Vis spectrum of the complex obtained in solution presented a characteristic d-d transition band at 685 nm which was not clearly observed in the solid state spectrum since there was a significant background between 500 – 800 nm. On the other hand, Raman spectrum revealed a γ(O–H) shift difference of about 10 cm^{-1} suggesting a chemical environmental change due to the metal coordination. Finally, the diffractogram of the mechanosynthesis sample showed a low degree of crystallinity with intensity changes and some peak shifts regarding to the $CuSO_4$ and β-CD patterns. These results pointed to a possible interaction between the ion and β-CD cavity. Electronic circular dichroism and mass spectrometry are underway in order to obtain further evidence of the complex formation in solid state.



Structure proposed in the literature

Acknowledgements: Authors acknowledge the brazillian financial agencies (FAPERJ, CNPq and CAPES) and CNRS.

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MDR - D3 - P01

Nitronyl nitroxide stable radicals derived from nitro-*o*-vanillin and bisphenol a as ligands towards 3d and 4f metal ions

Cristian Andrei Spinu[1,2], Daniel O.T. A. Martins[3], Teodora Mocanu[4], Mihaela Hillebrand[1], Gabriela Ionita[4], Ghenadie Novitchi[5], Floriana Tuna[3], Jean-Pascal Sutter[6], Marius Andruh[1,2]

[1]Faculty of Chemistry, University of Bucharest, Romania; [2]C.D. Nenitzescu Institute of Organic and Supramolecular Chemistry (ICOS), Romanian Academy, Romania; [3]Dept. of Chemistry and Photon Science Institute, University of Manchester, UK; [4]Ilie Murgulescu Institute of Physical Chemistry (ICF), Romanian Academy, Romania; [5]The Laboratoire National des Champs Magnétiques Intenses (LNCMI), CNRS, University Grenoble Alpes, France; [6]Laboratoire de Chimie de Coordination du CNRS (LCC), University of Toulouse, CNRS, France

Heterospin compounds may be synthesized using stable radicals and metal ions.[1] The nitronyl nitroxide organic radical derived from nitro-*o*-vanillin with 3d (Mn, Co, Ni, Zn) and 4f (Gd, Tb, Dy) metal ions led to 2p-3d, 2p-4f and 2p-3d-4f heterospin complexes while the diradical derived from bisphenol A with 3d (Co, Ni) metal ions led to 2p-3d heterospin complexes.[2,3,4] The structures of the obtained compounds have been solved by single-crystal x-ray diffraction and investigated by X-ray powder diffraction, elemental analysis, mass spectrometry and spectroscopic techniques (IR, UV-Vis). The cryomagnetic studies have revealed a strong magnetic interaction within the molecules, results which are sustained by theoretical DFT calculations. The mononuclear nickel and zinc complexes containing the nitronyl nitroxide derived from nitro-*o*-vanillin were investigated through pulse EPR to determine the spin-lattice relaxation time, T_1, and phase memory time, T_m, probing the qubit properties.

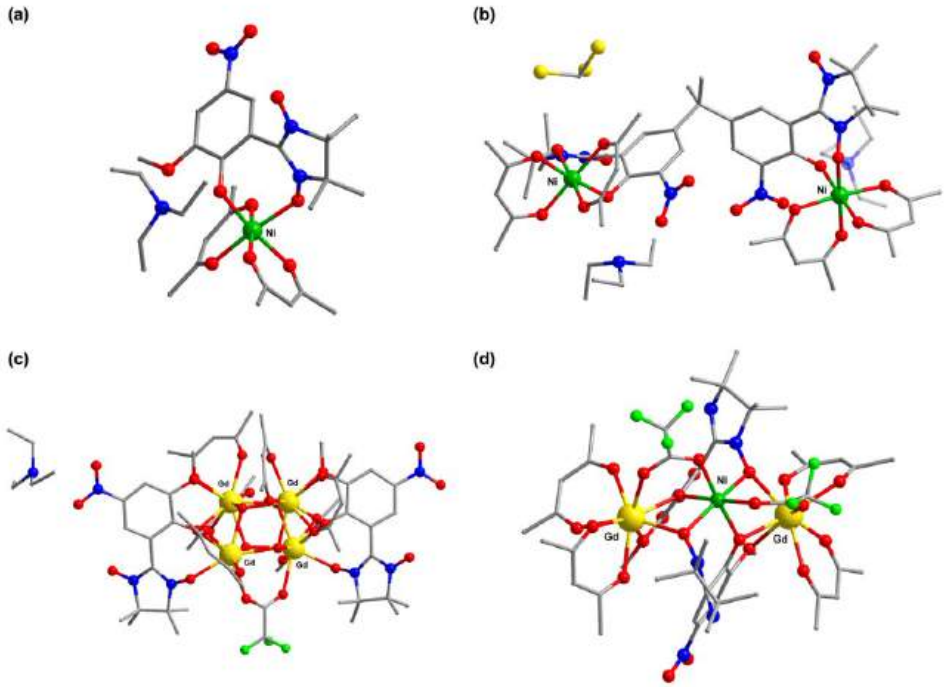

Fig. 1. Crystal structure of (a), (b) 2p-3d, (c) 2p-4f and (c) 2p-3d-4f heterospin complexes.

This work was supported by a grant from Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV and from European Union through NextGeneration EU-PNRR-III-C9-2022-I8 program (contract no. 760230).

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MDR - D3 - P02

Synthesis of steroidal and non-steroidal phase I and II metabolites relevant for doping analysis

Pia Gartlgruber[1], Nicolas Kratena[1], Günter Gmeiner[2], Peter Gärtner[1]

[1]Institute of Applied Synthetic Chemistry, Technische Universität Wien, Austria; [2]Doping Control Laboratory, Seibersdorf Labor GmbH, Austria

The abuse of performance enhancing drugs has been an issue since the invention of competitive sports. With the advent of modern biochemistry the potential performance gain was ever increased, for example by stimulants, anabolic agents and growth hormones.[1,2]

As the identification of doping agents is vital to prove this kind of substance abuse in professional athletes, metabolic studies are required to determine which metabolites are most prominent and preferably detectable over long periods of time. Metabolites are often oxidised, reduced, hydrolysed, and hydrated (phase I metabolism) or glucuronidated and sulphated compounds (phase II metabolism), transforming the doping agent into a less toxic, often less active and more hydrophilic form.[3-5]

In this work, we present the syntheses of various steroidal and non-steroidal phase I metabolites, including complex tamoxifen, DHCMT (Dehydrochloromethyltestosterone), and Oxymesterone metabolites, as well as phase II metabolites, Adrafinil, Hydrafinil, Andarine, and Epi-Trenbolone glucuronides, which required extensive studies of several glucuronidation methods (see Figure 1).

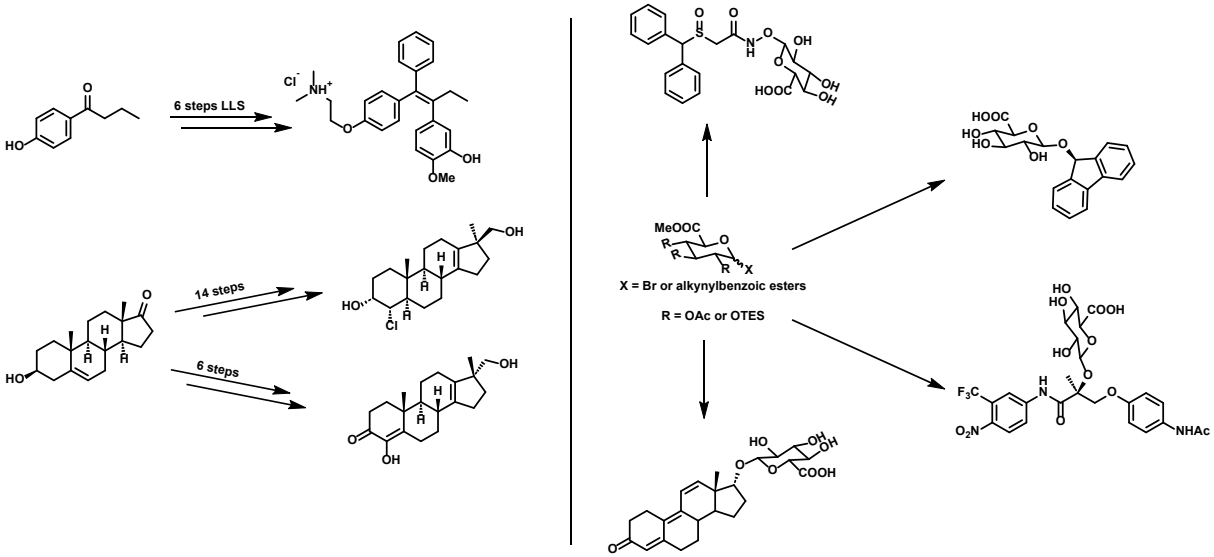

Fig. 1. Syntheses of phase I and II metabolites

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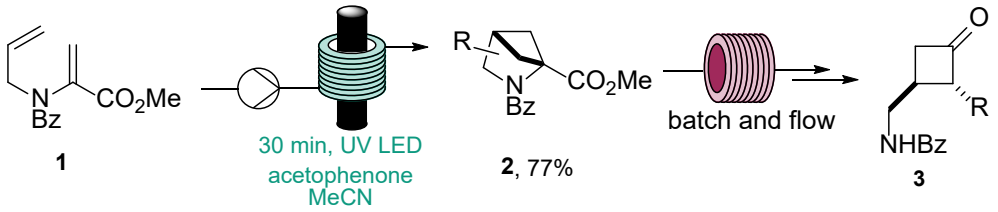
MDR - D3 - P03

Interrupted thermal rearrangement to access cyclobutanones via photochemistry and continuous flow chemistry

Daniel Corcoran[1], Marcus Baumann[1], Kian Donnelly[2]
[1]University College Dublin, Ireland; [2]SK Biotek, Ireland

Cyclobutanes are being increasingly used in medicinal chemistry in the search for building blocks with relevant biological properties.[1] Cyclobutanones have shown to be useful entities in organic synthesis due to their inherent ring strain and low activation barrier which allows for functionalisation at every position of the ring.[2,3] This work reports on an efficient synthesis of a functionalised cyclobutanone via photochemistry and an innovative thermal rearrangement, leveraging the intrinsic benefits of continuous flow chemistry.[4,5]
Compound **2** was accessed in continuous flow in 77% yield via a [2+2]-cycloaddition by irradiation of **1** with either 330 or 365 nm light, using acetophenone as a triplet sensitiser (Scheme 1). This scaffold is then transformed into the desired cyclobutanone scaffold via sequence of thermal reactions that exploit both batch and continuous flow processing. This new approach provides not only an attractive entry to drug-like cyclobutene building blocks, it also showcases how the union of thermal and photochemical transformations leverages a safe and potentially scalable entry into these industrially important scaffolds.



Scheme 1. Continuous flow photochemical synthesis of bridged pyrrolidine **2** and related cyclobutanones.

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MDR - D3 - P04
Novel 4,5-diphenyl-1,2,3-triazolate-based Kuratowski complexes with chiral active sites

Nikola Savic[1], Dirk Volkmer[1]
[1]University of Augsburg, Chair of Solid State & Materials Chemistry, Germany

The versatile coordination modes of 1,2,3-triazolate ligands have enabled their use in the synthesis of various metal complexes and metal–organic frameworks (MOFs)[1]. Pentanuclear Kuratowski complexes[2] hold a central octahedral metal ion (coordinated by six 1,2,3-triazolates), and four peripheral metal ions that bear suitable side-ligands. Tunable metal centers, counterions, and ligand substituents allow precise control over the electronic and steric environment of the active metal sites, which enable the activation of small molecules and catalysis[3-6].
We report on the synthesis and characterization of novel Kuratowski complexes based on 4,5-diphenyl-1,2,3-triazole (dphtH) ligands. Such complexes serve as well-defined model systems for structurally related MOFs, enabling the direct transfer of valuable insights from homogeneous to heterogeneous catalysis. In contrast to benzotriazole-based Kuratowski complexes that can form either penta- or nonanuclear compounds[7,8], the new ligand is sterically programmed to yield pentanuclear complexes exclusively and a chiral environment at the peripheral metal centers. This demonstrates how the defined geometries of the metal centers, which enable enzyme-like reactivities, can be further leveraged to enhance catalytic selectivity. Employing different transition metals, we obtained Kuratowski complexes featuring a variety of side ligands. For instance, organometallic Kuratowski complexes form spontaneously at high yield and under mild conditions with $Zn(alkyl)_2$ precursors. The reactivity of such complexes is currently investigated for nucleophilic addition reactions.

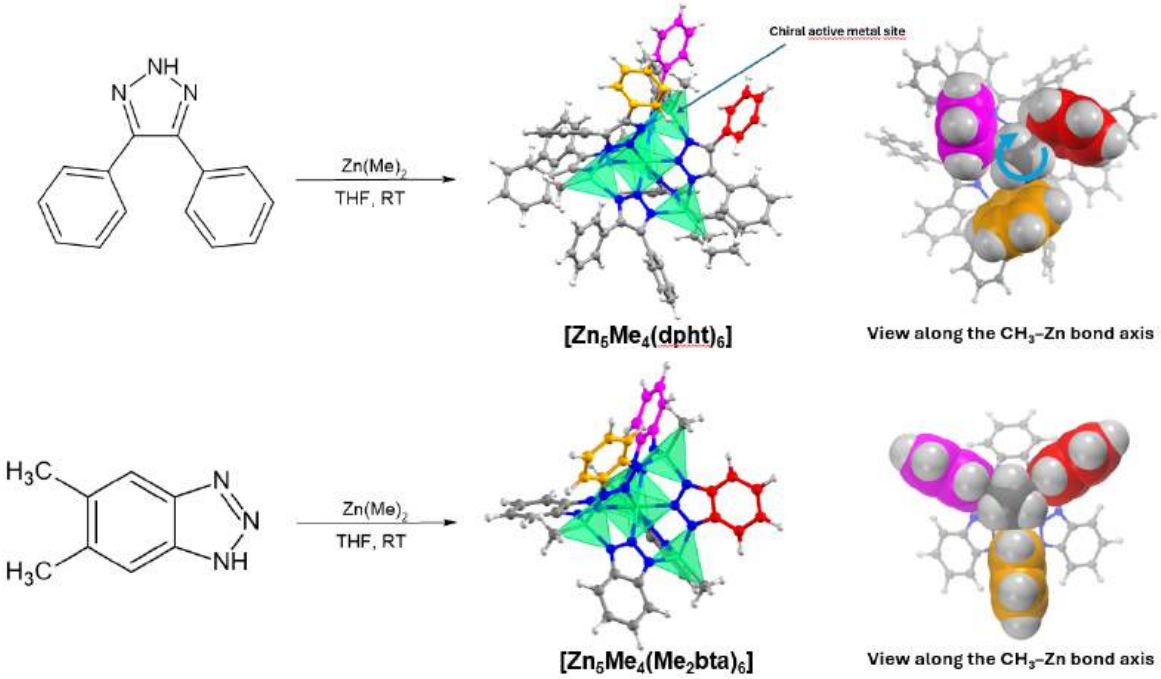

Fig. 1. Synthesis of Kuratowski complexes $[Zn_5Me_4(dpht)_6]$ and $[Zn_5Me_4(Me_2bta)_6]$

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MDR - D3 - P05
Regio- and stereoselective formation of 1,3-diols

Nick Kocem, Andreas Gansäuer
University of Bonn, Germany

Polyketides constitute a large and structurally diverse class of secondary metabolites exhibiting a wide range of biological activities, including antibacterial, antifungal, anticancer, antiviral, immunosuppressive, hypocholesterolemic, and anti-inflammatory effects.[1] Polyols featuring a 1,3-arrangement of hydroxyl groups represent a prominent subclass within this family. To enable their efficient synthesis, *Gansäuer* and co-workers developed a modular strategy for the construction of polyol chains with defined 1,3-hydroxyl spacing.[2] This approach starts from readily available allyl alcohols, which are transformed into glycidols *via* asymmetric *Sharpless*[3] epoxidation, followed by oxidation (e.g., *Swern*[4] oxidation) and a second asymmetric step using catalyst-controlled allylation as described by *Antilla*[5].
Building on this strategy, we developed a fluoride-mediated hydrosilylation method for the regio- and stereoselective opening of epoxides. The reaction employs phenylsilane as the reducing agent and *tert*-butylammonium fluoride (TBAF) as a fluoride source. This methodology enables the efficient synthesis of 1,3-diols with high diastereomeric and enantiomeric purity, as demonstrated in Figure 1. Ongoing studies focus on expanding the substrate scope, particularly with respect to substitution at the 1- and 2-positions.

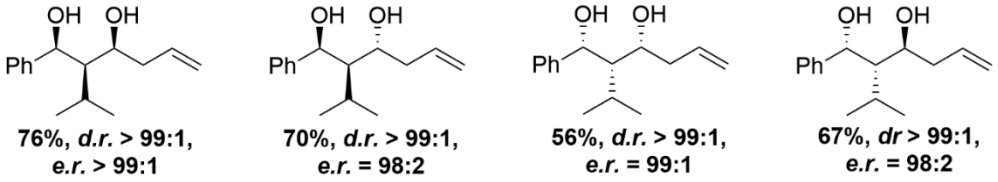

Fig. 1. Four stereoisomers of 1,3-diols obtained using our polyol synthesis.

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MDR - D3 - P06

Identifying promising low-fluorine weakly coordinating anions for lithium-ion batteries via high-throughput screening

Martin Hutereau[1], Yoann Olivier[1]
[1]Université de Namur, Belgium

In the drive for decarbonisation motivated by global warming, lithium-ion batteries (LIBs) have become ubiquitous, as best seen in the transport and energy sectors. However, most commercial batteries make use of electrolyte solutions containing $LiPF_6$ as the lithium salt.[1] This can degrade into toxic hydrofluoric acid in the presence of water,[1] degrading battery lifetime and presenting risks for end-of-life recycling. Our work aims to resolve this by identifying weakly coordinating anions with a lower fluorine content but comparable performance to commercial references. Inspiration can be drawn from known anions containing B,[2] Al,[3] or P atoms as the charged centres.[4] We first collected lithium salts based on these elements from the Cambridge Structural Database and Novel MAterials Discovery (NOMAD) repositories; while not novel, these may not have been studied in the context of LIBs. This set of anions was augmented by permuting atom types and substituting functional groups to reach over 2000 candidates. A high-throughput approach has been designed and deployed to evaluate key electrochemical properties at the density functional theory level: redox potentials for stability and the dissociation energy of the $[Li_n]^{n+}[anion]^{n-}$ complex as a proxy for lithium mobility. This allowed for a first sifting based on performance relative to $LiPF_6$, leaving behind 10% of the initial structures. Subsequent screening with more detailed calculations narrowed these further to 12 distinct families of anions, minimising the synthesis and characterisation workload of our experimental partners.

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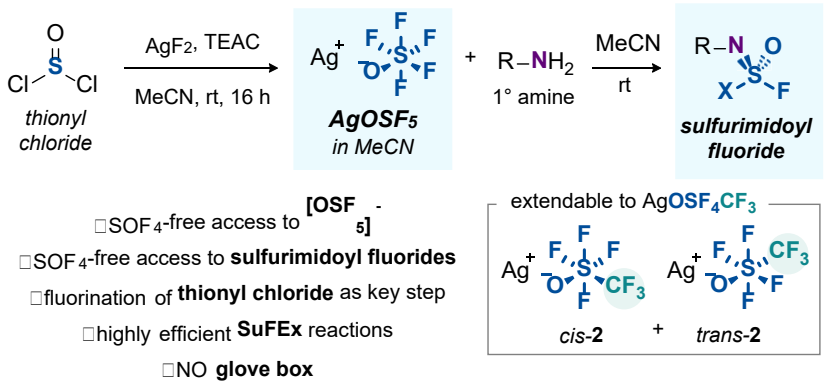
MDR - D3 - P07

Perfluorooxosulfate salts as SOF_4-gas-free precursors to multidimensional SuFEx electrophiles

Armir Zogu, Karim Ullah, Stefanos Spanopoulos, Ermal Ismalaj, Wim M. De Borggraeve, Joachim Demaerel
Dept. of Chemistry, Sustainable Chemistry for Metals and Molecules (SCM²), KU Leuven, Belgium

Sulfur(VI) Fluoride Exchange (SuFEx) chemistry stands as a well-established method for swiftly constructing complex molecules in a modular fashion. An especially promising segment of this toolbox is reserved for multidimensional SuFEx hubs: three or more substituents pluggable into a singular S^{VI} centre to make 'beyond-linear' clicked constructions. Sulfurimidoyl difluorides ($RNSOF_2$) stand out as the prime example of this, however their preparation from the scarcely available thionyl tetrafluoride (SOF_4) limits this chemistry to only a few laboratories with access to this gas. In this work, we identify silver pentafluorooxosulfate ($AgOSF_5$) as a viable SuFEx hub with reactivity equal to SOF_4. The AgF_2-mediated oxidation of $SOCl_2$ gives rise to the hexacoordinate $AgOSF_5$ adduct, which in contact with primary amines produces the sulfurimidoyl fluorides in high yields. In addition, we have found this workflow to be fully extendable to the trifluoromethyl homologue, $AgOSF_4CF_3$, and we propose the use of $AgOSF_4X$ salts as a general route to azasulfur SuFEx electrophiles from commercial starting materials (scheme 1)[1].



Scheme 1. $AgOSF_4X$ salts as a SuFEx reservoir

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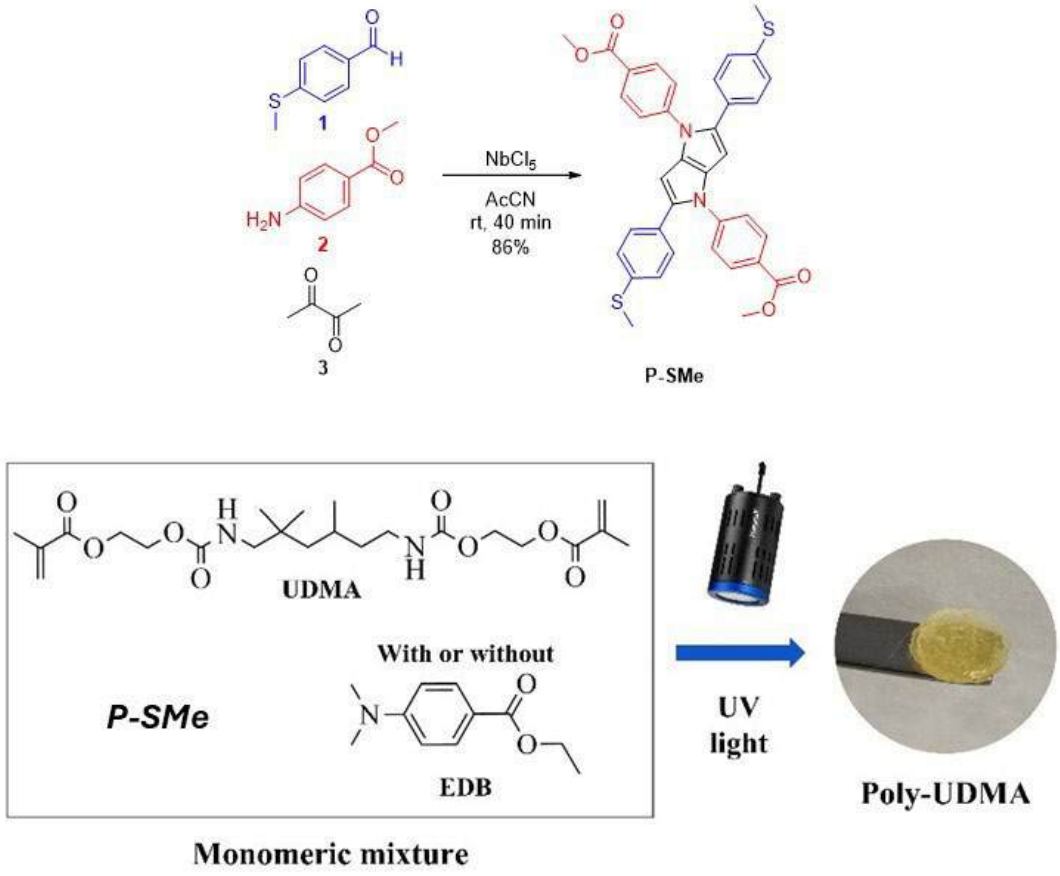
MDR - D3 - P08

Expanding visible-light photopolymerization: Azapentalene derivatives for methacrylate and biobased acrylic systems

Ilana Sganzerla Rosário[1], Caroline Gaglieri[1], João Antônio Ribeiro Bassetto[1], Luiz Carlos da Silva-Filho[1*]
[1]São Paulo State University (UNESP), School of Sciences, Dept. of Chemistry, Bauru, Brazil

The global UV-curable resins market—surpassing 380,000 metric tons and USD 6.63 billion in 2024—highlights the industrial criticality of photopolymerization.[1] However, transitioning from UV to lower-energy visible light (430 nm) requires novel photoinitiator systems (PISs), as most commercial radical initiators lack absorption in the visible spectrum.[2] This study investigates a newly synthesized azapentalene derivative (P-SMe) as a PI for the polymerization of urethane-dimethacrylate (UDMA) and acrylated macaw vegetable oil (AMWO), a sustainable bio-monomer.[3] Photopolymerization experiments were performed using 0.5 wt% of P-SMe as PI in the presence or absence of ethyl-4-(dimethylamino)benzoate (EDB, a co-initiator) (Figure 1). The conversion of monomeric mixture into polymer (MC%) and the rate of polymerization (Rp) were determined by mid-infrared spectroscopy.[4] Although the systems without EDB resulted in MC% values below 30%, its presence led to higher values, with UDMA system exhibiting the highest one (MC% = 51.0 ± 3.0%). Both systems reached maximum Rp at around 20 seconds, indicating their potential for use in vat photopolymerization after optimization of processing conditions Thermal characterization via TG/DTG-DTA established stability thresholds of 213.0 °C and 196.0 °C for UDMA and AMWO polymers, respectively. Furthermore, differential scanning calorimetry (DSC) confirmed the absence of exothermic events prior to degradation, indicating no residual thermal polymerization. Qualitative analysis also revealed intrinsic luminescence under UV light in the resulting polymers. These findings demonstrate that azapentalene derivatives are effective candidates for visible-light photopolymerization, yielding thermally stable and functional materials.



The authors would like to thank FAPESP [Grant numbers 2024/02435-1, 2024/00779-2, 2024/02935-1, 2025/27044-5), CNPq [Grant number 303750/2024-3] and CAPES.

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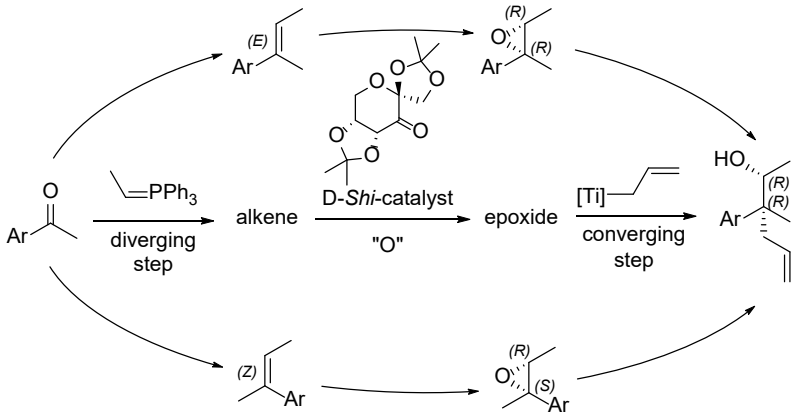
MDR - D3 - P09

Stereoconvergent approach to the enantioselective construction of *α*-quaternary alcohols by radical epoxide allylation

Annika Plato[1], Sebastian Höthker[1], Andreas Gansäuer[1], Zheng-Wang Qu[2], Stefan Grimme[2]
[1]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Germany; [2]Mulliken Center for Theoretical Chemistry, Universität Bonn, Germany

Numerous biologically active natural products and pharmaceutical agents contain all-carbon quaternary stereocenters (ACQS). Representative examples such as Naloxone (opioid antagonist), Strychnine (neurotoxin), and Haemanthamine (cytostatic) highlight the importance of efficient strategies for their enantioselective construction. Although several approaches exist, they often require stereodefined olefinic substrates.[1]

We developed a straightforward approach to access a single *α*-quaternary alcohol from a diastereomeric mixture of the corresponding olefin *via Shi* epoxidation followed by stereoconvergent titanocene-promoted radical epoxide allylation.[1] Therefore, a stereodivergent olefination method, such as the *Wittig* olefination, is sufficient for the preparation of the substrates. The following *Shi* epoxidation establishes the absolute configuration at the less substituted carbon regardless of the olefin's geometry with equally high selectivity. Subsequently, the diastereoconvergent titanocene-promoted radical epoxide allylation furnishes the enantiomerically and diastereomerically enriched *α*-quaternary alcohol. In this process, we employed $Cp_2Ti(III)$allyl as the active species, which is generated *in situ via* transmetalation of benchstable Cp_2TiCl_2 with MgCl-allyl. This species induces homolytic cleavage of the C–O bond *via* single-electron transfer affording the benzylic *β*-titanoxy radical. Consequently, the initial stereoinformation of the higher substituted carbon is lost. The resulting radical rotamers can interconvert *via σ*-bond rotation prior to the *syn*-selective allyl transfer. Thereby, the allyl transfer proceeds exclusively *via* the favored transition state, facilitating the underlying diastereoconvergence.



Scheme 2. Stereoconvergent approach towards *α*-quaternary alcohols.

This method provides an efficient route to enantioenriched *α*-quaternary alcohols with broad substrate scope, good yields and high diastereoselectivity, expanding the toolbox for asymmetric synthesis of complex molecular architectures.

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MDR - D3 - P10

Design and synthesis of N-formyl/carbothioamide based pyrazoline analogs using $Pd(PPh_3)_4$ catalyst: Cytotoxicity, apoptosis, and molecular dynamics studies

Manish Rana[1], Imran Ansari[2], Sumbul Khan[2], Rabiya Mehandi[3], Rahis Uddin[3]
[1]Dept. of Chemistry, Ramjas College, University of Delhi, New Delhi, India; [2]Special Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi, India; [3]Molecular and Biophysical Research Laboratory (MBRL), Dept. of Chemistry, Jamia Millia Islamia, New Delhi, India

To expand the scope of our research and find anticancer drugs with novel structures, heterocyclic derivatives (**3a-3n**) were designed and synthesized via Suzuki coupling reaction in the presence of Pd(PPh3)4 [Tetrakis(triphenylphosphine)-palladium(0)] catalyst with good yields. The synthesized heterocyclic analogs were characterized using various spectroscopic techniques like 1H, 13C NMR, and FT-IR spectroscopy. The cytotoxicity of heterocyclic analogs (**3a-3n**) was carried out by MTT assay towards breast cancer cell (**MCF-7**), and human normal cells (**HepG2**), analog **3j** exhibited excellent activity against an MCF-7 (**IC_{50} = 5 ± 1.58 µM**) and low toxicity against the HepG2 (**IC_{50} = >80 µM**).

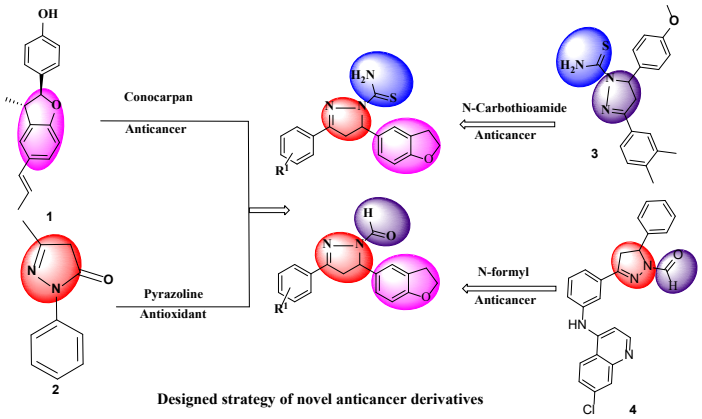

Fig.1. The designed strategy of novel compound.

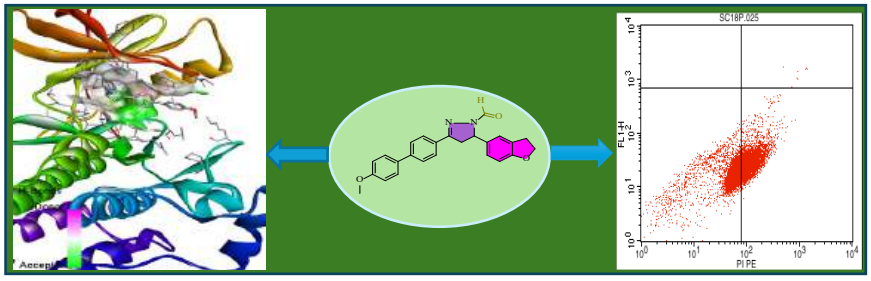

Fig. 2. The structure of active heterocylic compound.

Furthermore, the anticancer activity of lead analog against the MCF-7 cancer cell line was confirmed using flow cytometry. Molecular dynamics study revealed that the derivative fits well at the active site of the target protein epidermal growth factor receptor tyrosine kinase. The designed strategy and structure of lead comounds has shown in **Fig.1** and **2**.

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MDR - D3 - P11
Triplex DNA clamp regulates Cas12a activation for ssDNA and RNA sensing

Andrea Celeste Di Pede[1], Neda Bagheri[1], Erica Belforte[1], Alessio Palone[1], Marianna Rossetti[1,2], Alessandro Porchetta[1]
[1]Dept. of Chemical Science and Technologies, University of Rome, Tor Vergata, Rome, Italy; [2]Nanobioelectronics & Biosensors Group, Catalan Institute of Nanoscience and Nanotechnology(ICN2), CSIC and BIST, Campus UAB, Bellaterra Barcelona, Spain

The widespread use of CRISPR technologies in molecular diagnostics has been enabled by the discovery of collateral, non-specific cleavage activities exhibited by type V (Cas12) and type VI (Cas13) CRISPR systems upon DNA or RNA target recognition.[1] In particular, Cas12 is an RNA-guided endonuclease that integrates single- and double-stranded DNA recognition with collateral cleavage, which can be harnessed for signal generation through the Cas12-mediated digestion of fluorophore–quencher-labeled hairpin DNA reporters.[2]
Here we present a strategy to control Cas12a cleavage activity through a rationally designed DNA-based hybridization network built on Triplex Clamp formation.[3] This approach takes advantage of a clamp-like binding mechanism that ehnances both the specificity and the affinity of homopurine DNA or RNA recognition through triplex folding. Within this framework, we developed a DNA hairpin, called the PAM-Switch, that controls Cas12a activation and triggers fluorescence signal generation. By decoupling target recognition from direct hybridization with the Cas12a–crRNA complex, this approach eliminates the need for target-specific crRNAs and allows multiple parallel detection of distinct nucleic acid sequences using a single CRISPR reaction mix. Furthermore, triplex-based clamps enhance single-nucleotide variant discrimination and enable detection of short ssDNA and RNA targets (10–20 nucleotides). Overall, this platform addresses some of the most relevant limitations of existing Cas12a-based diagnostic platforms and provides a versatile framework for nucleic acid sensing.

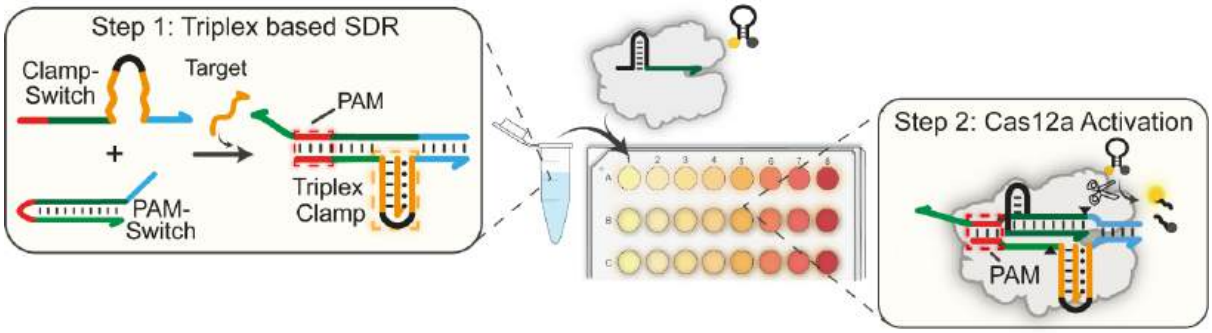

Fig. 1. Schematic representation of the two-step sensing strategy. In step 1 (left), target recognition triggers a triplex-based strand displacement reaction, leading to the formation of the Triplex Clamp that enables reconfiguration of the PAM-Switch and exposure of the PAM motif. In step 2 (right), PAM availability allows Cas12a activation, resulting in collateral cleavage and generation of a measurable fluorescent signal.

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MDR - D3 - P12
Investigation of a low-valent molybdenum complex towards reductive N_2-activation

Niels Michaelis[1], Tobias A. Engesser[1], Jan Krahmer[1] and Felix Tuczek[1]
[1]Christian-Albrechts-Universität zu Kiel, Germany

The production of NH_3 and other N-containing building blocks from elemental N_2 (N_2RR) has always attracted researchers due to its importance as industrial feedstock.[1] Demand in efficient NH_3 production is anticipated to increase due to its potential role in the storage and shipment of H_2.[2] Current state of the art transition-metal halide pre-catalysts feature tridentate pincer type ligands that achieve up to 60.000 equivalents of NH_3 per run.[3] A key intermediate in the catalytic cycle is the *in situ* formation of a (L)M-N≡N-M(L) dimer under reductive conditions, facilitating N_2-scission into two (L)M≡N nitrides.[4] Whereas NN-cleavage is understood in terms of stabilizing a certain electron number inside the M-N≡N-M scaffold,[5] the role of the supporting ligand and its terminal PR_2 donors (R = ^{t}Bu, ^{i}Pr, Cy) is less clear.[6] Herein, we report the synthesis and characterization of a new PPP pincer type ligand bearing cyclopentyl substituents (PPP^{Cyp}) together with the potential pre-catalyst [$MoBr_3(PPP^{Cyp})$]. With this platform at hand, we investigated its capabilities towards reductive N_2-activation by means of experimental and theoretical methods. Our results provide important insights for further ligand development tailored towards N_2RR.

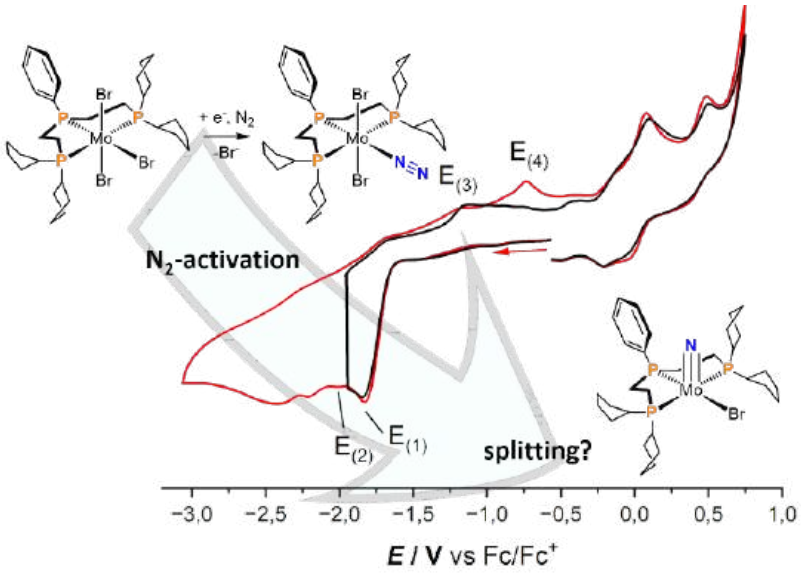

Fig. 2. CV of 1 mM [$MoBr_3(PPP^{Cyp})$] in 0.1 M $TBAPF_6$/abs. THF under N_2-atm. as survey- (red) scan at 0.1 V/s. $E_{(1)}$ and $E_{(2)}$ depict correspond to the reduction to the Mo^I and Mo^0 state. Limiting the scan to $E_{(1)}$ and holding the potential for 30 sec (black), a new species at $E_{(3)}$ arises. Graphical inset depicts the first EC-step for reductive N_2-activation (E = electrochemical, C = chemical) at the potential $E_{(1)}$.

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MDR - D3 - P13

Investigation of mononuclear molybdenum and tungsten complexes with pentaphosphine environment for activation of dinitrogen and catalytic ammonia synthesis

Anna-Marlene Vogt[1], Tobias A. Engesser[1], Jan Krahmer[1] and Felix Tuczek[1]
[1]Christian-Albrechts-Universität zu Kiel, Germany

Synthetic nitrogen fixation is a highly competitive and challenging research area focused on achieving a fundamental understanding of activating N_2 and its subsequent conversion into NH_3.[1-3] Inspired by the enzyme nitrogenase, molybdenum-dinitrogen complexes have emerged as effective chemocatalysts for N_2-to-NH_3 catalysis.[1-4, 7] In contrast, experimental attempts with tungsten were less successful, even though N_2 bound in tungsten complexes appears to be more activated.[5-7] We developed a ligand scaffold for N_2 activation and NH_3 catalysis based on a pentadentate tetrapodal phosphine ligand (pentaPod, P5) bearing dimethylphosphino ($P5^{Me}$) or phospholano ($P5^{Pln}$) groups.[4-6] The molybdenum complexes [Mo(N_2)$P5^{Me}$] and [Mo(N_2)$P5^{Pln}$] generate 26 respectively 22 equivalents of NH_3 from N_2 under optimized conditions. The complex [W(N_2)$P5^{Me}$] produces 2.5 and surprisingly [W(N_2)$P5^{Pln}$] generates 7 equivalents of NH_3, rendering the latter the first tungsten complex chemocatalytically converting N_2 to NH_3.[4-6] The reason for this difference in reactivity and the impact of the pentaPod topology has not been fully understood.[6,7] Owing to their unique topology and modular design, pentaPod ligands enable systematic structural variation and fine-tuning of the overall ligand scaffold to investigate N_2 activation and catalysis.[7]

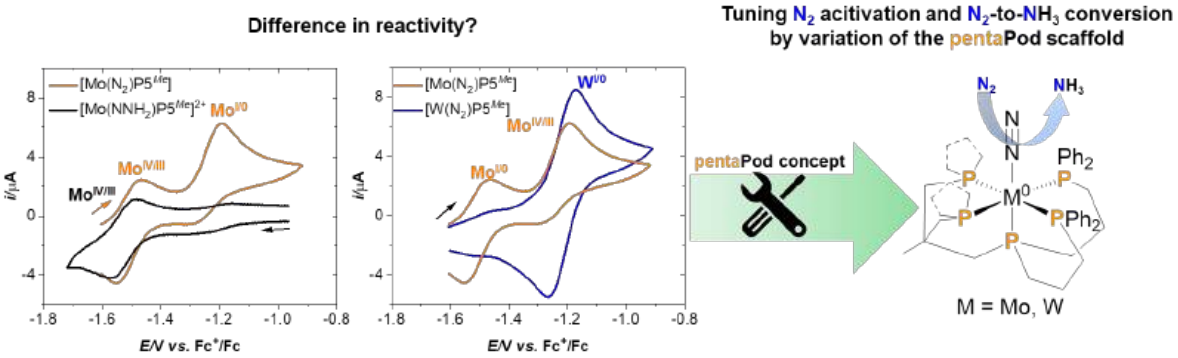

Fig. 1. Cyclic voltammetry (CV) studies of pentaPod complexes [M(N_2)$P5^R$] (M = Mo, W; R = Me, Pln) suggest a difference in reactivity (left); variation of the pentaPod ligand offer possibilities for optimization and investigation of N_2 activation and NH_3 synthesis with molybdenum and tungsten complexes (right).

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MDR - D3 - P14

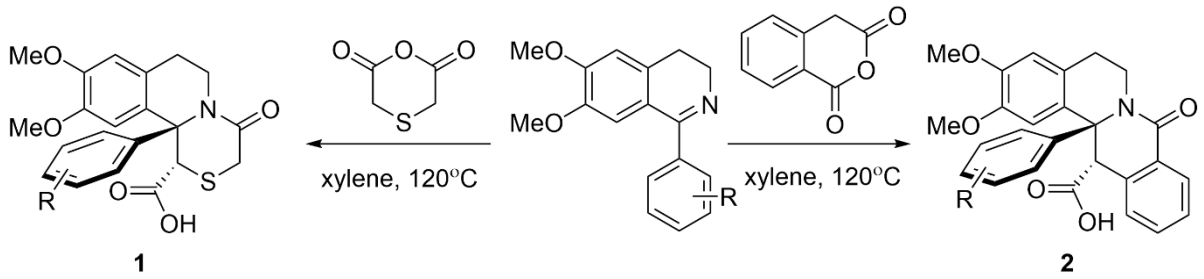
Angular substituted dibenzo[a,g]quinolizidines – synthesis and DPP-IV inhibitory activity

Aleksandar Pashev[1], Valentin Petrov[1], Elena Todorova[1], Asya Milozinova[1], Lidiya Petrova[2], Milena Atanasova[2], Teodora Aleksandrova[1]

[1]Faculty of Pharmacy, Medical University Pleven, Bulgaria; [2]Faculty of Medicine, Medical University Pleven, Bulgaria

Recent studies have discovered that aryl-substituted benzo[a]quinolizidines have the potential to be highly active DPP IV inhibitors[1]. In previous studies, we reported a novel synthetic approach for the construction of their sulfur-containing bioisosteric [1,4]thiazino[3,4-a]isoquinolines analogues **1**, incorporating an additional aryl substituent[2]. The target compounds are obtained via a one-step reaction between cyclic imines and enolizable cyclic anhydrides. Further in vitro studies of the obtained compounds **1** identified that three compounds demonstrated IC_{50} in the mid-micromolar range, with the lead compound (IC_{50} = 0.35 μM) bearing a *p*-fluorophenyl substituent[3]. These results are comparable to the inhibitory activity of various natural and synthetic DPP-IV inhibitors published in recent years.

Building on these results, we focused on using our approach to construct novel dibenzo[*a,g*]quinolizidines **2** and to test their DPP-IV inhibitory activity. This could give rise to previously unexplored heterocyclic motifs to be used as DPP-IV inhibitors. The heterocyclic fragment in compounds **1** and **2** is rarely found in the recent literature, which makes them interesting from a synthetic and medicinal chemical point of view.



1 **2**

Fig. 1. Synthesis of target compounds.

This study is financed by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0003.

[1] Petrov, V; Aleksandrova T.; Pashev, A, *Molecules* **2025**, 30(5), 1043; doi: 10.3390/molecules30051043

[2] Pashev, A.; Burdzhiev, N.; Stanoeva, E. *J. Heterocycl. Chem*. **2023**, 60, 513-518, doi:10.1002/jhet.4601

[3] Pashev, A.; Petrov, V.; Pesheva, A.; Petrova, L.; Ilieva, K.; Stavreva, G.; Atanasova, M.; Cheshmedzhieva, D.; Altankov, G.; Aleksandrova, T. *Int J Mol Sci* **2024**, 25, 11753, doi:10.3390/ijms252111753

MDR - D3 - P15

Novel heterocyclic derivatives based on the [1,4]thiazino[3,4-a]isoquinoline ring system – Molecular design, synthesis and DPP-IV inhibitory activity

Aleksandar Pashev[1], Valentin Petrov[1], Elena Todorova[1], Asya Milozinova[1], Lidiya Petrova[2], Milena Atanasova[2], Teodora Aleksandrova[1]

[1]Faculty of Pharmacy, Medical University Pleven, Bulgaria; [2]Faculty of Medicine, Medical University Pleven, Bulgaria

Dipeptidyl Peptidase IV (DPP-IV) inhibitors are extensively studied as a treatment of type 2 diabetes with eleven inhibitors currently approved and many more in development. Previous studies have identified aryl-substituted benzo[a]quinolizidines as prospective DPP-IV inhibitors[1].

Earlier studies in our group were focused on the development of a one-step approach toward the benzo[a]quinolizidine system and its heterocyclic analogs based on the reaction between enolizable anhydrides and 3,4-dihydroisoquinolines[2]. The binding mode of the previously synthesized compounds at the active site of the human DPP-IV enzyme was further explored using molecular docking. The obtained results were used to guide the structure optimization process. Based on this, two series of potential DPP-IV inhibitors were synthesized, incorporating an aryl-substituted benzo[a]quinolizidine fragment[3].

The inhibitory activity of the synthesized compounds against human DPP-IV was measured using Sitagliptin as a positive control. Several of the compounds were found to possess inhibitory activity in the micromolar range. The cytotoxic activity on human mesenchymal stem cells was evaluated, with all compounds showing no cytotoxic activity at micromolar concentrations.

In conclusion, the molecular docking approach allowed us to successfully optimize the structure of the benzo[a]quinolizidine inhibitors and to outline the necessary modifications to increase their potency as DPP-IV inhibitors. This synthetic methodology could provide a route to previously unexplored heterocycles with potential biological properties.

This study is financed by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0003.

[1]Petrov, V; Aleksandrova T.; Pashev, A, *Molecules* **2025**, 30(5), 1043; doi: 10.3390/molecules30051043
Pashev, A.; Burdzhiev, N.; Stanoeva, E. *J. Heterocycl. Chem.* **2023**, 60, 513-518, doi:10.1002/jhet.4601
[3]Pashev, A.; Petrov, V.; Pesheva, A.; Petrova, L.; Ilieva, K.; Stavreva, G.; Atanasova, M.; Cheshmedzhieva, D.; Altankov, G.; Aleksandrova, T. *Int J Mol Sci* **2024**, 25, 11753, doi:10.3390/ijms252111753

MDR - D3 - P16

Water-soluble acylgermanes via a Germa–Michael Reaction: A modular route toward bio-compatible photoinitiators

André Culum[1,2], Matthias Paris[1], David Vorcnik[1], Renata Raptova[3], Georg Gescheidt[3], Tanja M. Wrodnigg,[2] Michael Haas[1]

[1]*Institute of Inorganic Chemistry, Graz University of Technology, Austria*; [2]*Institute of Chemistry and Technology of Biobased Systems, Graz University of Technology, Austria*; [3]*Institute of Physical and Theoretical Chemistry, Graz University of Technology, Austira*

Acylgermanes are efficient photoinitiators for free-radical polymerization but are typically limited to nonpolar or weakly polar systems due to poor water solubility.[1] At the same time, new bond-forming reactions that expand the synthetic toolbox of organogermanium chemistry remain scarce. Addressing both challenges, we report a modular and scalable strategy toward water-soluble acylgermanes that is enabled by a previously unexplored Germa–Michael addition.[2]

The synthetic strategy relies on the reaction of an acylgermane nucleophile (**1**) with α,β-unsaturated Michael acceptors (**2**), forming acylgermane adducts (**3**) via a Germa-Michael addition. This novel reaction affords air- and moisture-stable products in high purity on multigram scale. Depending on the nature of the Michael acceptor, the resulting compounds are either directly water-soluble or serve as highly versatile precursors for the introduction of hydrophilic or biologically relevant functionalities.

The resulting compounds (**3**) exhibit excellent solubility in water and aqueous solvent mixtures, readily reaching millimolar concentrations suitable for photopolymerization. In addition, cytotoxicity screenings were conducted, providing initial insights into the biological compatibility of these water-soluble acylgermanes.

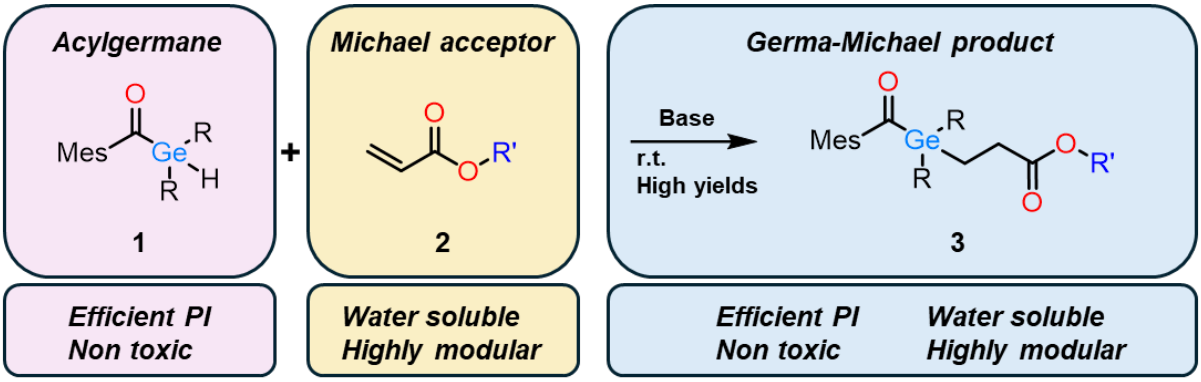


Fig. 3. Germa-Michael addition of an acylgermane (**1**) to a Michael acceptor (**2**) yielding Germa-Michael products (**3**). R' represents a water soluble or reactive functional moiety.

[1] Müller, S. M.; Schlögl, S.; Wiesner, T.; Haas, M.; Griesser, T. *ChemPhotoChem* **2022**, *6* (11), e202200091.

[2] EP25160048.2, Matthias Paris, Renata Raptova, André Culum, Georg Gescheidt, Michael Haas.

MDR - D3 - P17

The effect of PEG localization and charge density on transfection ability of artificial gene delivery vectors

Merve Ercan Ayra[1], Semih Macit[1], Osman Mersin[1], Yasemin Yuksel Durmaz[1,2]

[1]School of Engineering and Natural Sciences, Istanbul Medipol University, Turkey; [2]Research Institute of Health Science and Technologies (SABITA), Istanbul Medipol University, Turkey

Gene therapy is a promising tool for treatment of genetic diseases, immunogenic disorders, and cancer with reduced side effects and enhanced efficiency.[1] The key points for a gene delivery agent are targeting specific cells and ensure that the genetic cargo reaches the nucleus while keeping cargo-carrier complex stable in the route. In this study, polyethylene glycol (PEG) is used to keep the macromolecule for longer time in the system to prevent rapid clearance[2] and β-cyclodextrin (β-CD) is used to enable “click” chemistry through the seven azide groups. β-CD is modified with poly (hexyl methacrylate)-poly (2- (dimethyl amino) ethyl methacrylate)-poly (N,N,N-trimethyl aminoethyl methacrylate P(HMA-*co*-DMAEMA-*co*-TMAEMA) which is synthesized via atom transfer radical polymerization (ATRP), and PEG at different positions mainly. The carriers are prepared with different cationic charge density, molecular weight, hydrophobicity and PEG ratio. These carriers condensed with model gene GAPDH siRNA through electrostatic interaction. The GAPDH activity is found as 2.2-2.8 U/mL on breast cancer cells (MCF7). Moreover, cytotoxicity of the star polymers is found as less than 25% without PEG and less than 10% with PEG on epithelial human breast non-tumorigenic cells (MCF10A). The study shows that it is important to consider those alterations to design an ideal gene carrier with both efficient complexation behaviour and reduced harm in healthy tissue for contribution to development of novel gene therapies.

Keywords: macromolecular engineering, cationic polymers, non-viral vector.

Code	***Mw CP***	***#CP[a]***	***#PEG***	***#TMAEMA***	***N/P***
P1L	32135	6	0	47	4
P2L	32135	3,3	3,7	47	6
P3L	32135	6	10	47	6
P1M	27656	6	6	31	6
P2M	27656	3,6	3,4	31	4
P3M	27656	6	11	31	4
P1S	13656	6	0	19	4
P2S	13656	3,4	3,6	19	6
P3S	13656	6	11	19	2

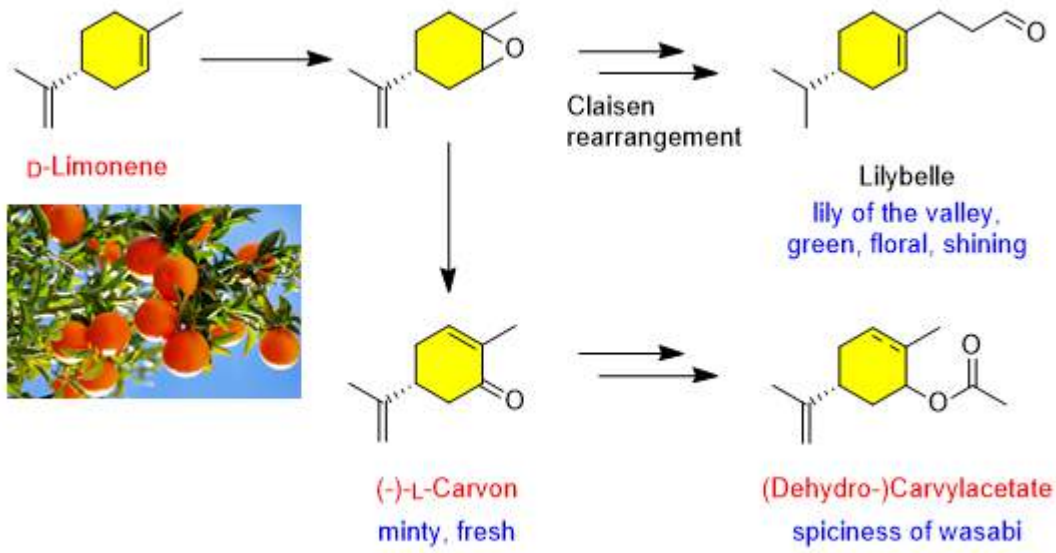
Table 1. Structural information of star polymers.
[a]Cationic Polymer.

[1]Mohammad, R. Key Considerations in Formulation Development for Gene Therapy Products. *Drug Discov. Today* **2022**, *27* (1), 292–303.
[2]Royo-Rubio, E.; Rodríguez-Izquierdo, I.; Moreno-Domene, M.; Lozano-Cruz, T.; de la Mata, F. J.; Gómez, R.; Muñoz-Fernández, M. A.; Jiménez, J. L. Promising PEGylated Cationic Dendrimers for Delivery of miRNAs as a Possible Therapy against HIV-1 Infection. *J Nanobiotechnol* **2021**, *19* (1), 158.

MDR - D3 - P19
From oranges to odorants: Using renewable starting materials for fragrance chemistry

Franziska Elterlein[1]
[1]*Symrise AG, Germany*

The demand for sustainability includes search for biodegradable materials, upcycling, safety of materials and processes, use of renewables and atom-economic reactions. In Flavor and Fragrance industry, a fragrance chemist's task is the design and synthesis of new odorants with effect in consumer applications ranging from fine fragrance perfumes to household and personal care products such as shampoo and body lotion. Regarding sustainability, especially the renewability of starting materials is of interest, as the origin of starting materials can be considered when synthesis planning.[1]
D-Limonene is obtained from the peel of oranges. It can be further transformed into L-carvone with its typical minty odor by epoxidation and reduction.[1,2] Carvone itself served as starting material for further reduction and esterification to give several carvylesters. Out of these, especially the acetate is of olfactive interest, giving a spicy impression as of wasabi. Therefore, it is used as odorant signature molecule impacting a fragrance creation.[2]
In another example, D-Limonene is oxidized to menthenole, a versatile substrate for further transformations. By Claisen rearrangement, Lilybelle, a floral, lily of the valley (muguet) odorant molecule was obtained.[3] No muguet odorant can be extracted from the flower itself and many synthetic muguet odorants have toxicological issues.[1] Lilybelle shows its beauty in being renewable, biodegradable and without use restrictions. Further chemical derivatives were synthesized to explore the chemical space and approach structure-activity understanding.



Scheme 1. Exemplified synthesis of odorants using D-Limonene originating from the peel of oranges as starting material.

[1]Elterlein, F.; Bugdahn, N.; Kraft, P. *Chem. Eur. J.* **2024**, *30*, e202400006.
[2]Hölscher, B.; Mansfeld, M.; Chmelnyk, A.; Siegel, S. (to Symrise), PCT Int. Pat. Appl. WO2017/041834 A1, 8 September, **2015**.
[3]Singer, E.; Hölscher, B. (to Symrise AG), Eur. Pat. Appl. EP 2 578 671 B1, 7 October, **2011**.

MDR - D3 - P20

A first principle study of a model bimolecular nucleophilic substitution reaction promoted by catalysts supported on oxidized carbon black

Maria Voccia[1], Rosaria Schettini[2], Maria Rosaria Acocella*[2], Sergio Tosoni*[1]
[1]Dept. of Materials Science, University of Milan-Bicocca, Italy; [2]Dept. of Chemistry and Biology "A. Zambelli" Chemistry, University of Salerno, Italy

In this work a study employing first-principles Density Functional Theory (DFT) calculations and Ab Initio Molecular Dynamics (AIMD) is reported to derive, for the first time, a model of oxidized carbon black (oCB) with an oxygen-to-carbon weight ratio of approximately 50%, Figure 1.
Recently, this oCB[1-3] has been employed as a heterogeneous support for ammonium and phosphonium salts used as phase-transfer catalysts and evaluated in S_N2-type reactions.[4-5]
To rationalize the experimental findings, adsorption studies of ammonium and phosphonium ions on different oCB surface sites were carried out. The model of oCB was then used to investigate the S_N2 reaction between sodium thiocyanate and benzyl bromide, catalysed by an ammonium salt, in aqueous media.[5]
The results demonstrate that the oCB support plays a crucial role in stabilizing reaction intermediates through hydrogen-bond interactions, while the quaternary ions act as effective mediators along the reaction pathway. These insights provide a molecular level explanation for the high catalytic activity observed and highlight oxidized carbon black as a efficient and reusable platform for phase-transfer catalysis reactions.

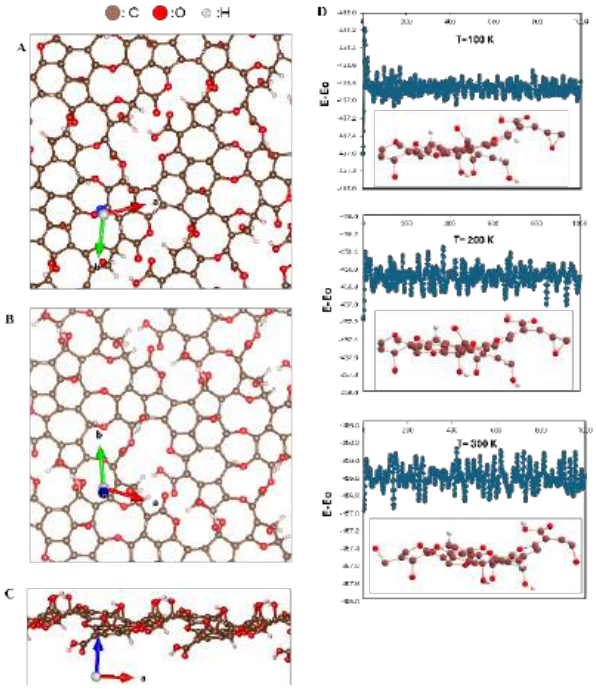


Fig. 1. The optimized oCB structure from both top (4A and 4B) and side views (4C) (gray atoms represent carbon, red atoms represent oxygen and light gray atom represent hydrogen). (4D) Variations in the gradient values of the total energies for the single oCB layer as a function of simulation time at the three different temperatures of AIMD.

[1]Schettini, R.; Acocella M.R.; *ChemCatChem* **2024**, e202301425.
[2]Kiani, A.; Acocella, M. R.; Granata, V.; Mazzotta, E.; Malitesta, C.; Guerra G.; *ACS Sustainable Chemistry & Engineering* **2022**, 10 (48), 16019-16026
[3]Acocella, M. R.; De Pascale, M.; Maggio, M.; Guerra, G.; *J. Mol. Catal. A: Chem.,* **2015**.
[4]Melillo, A.; Kiani, A.; Schettini, R.; Acocella, M. R.; *Molecular Catalysis* **2023**, 537, 112951.
[5]M. Voccia, R. Schettini, M. R. Acocella and S. Tosoni, *Catal. Sci. Technol.*, **2026**, DOI: 10.1039/D5CY00260E

MDR - D3 - P28

Malonic-type macrocyclic esters from catechol-derived propargyl diols: Effect of catechol substituents on reactivity

Savvas N. Georgiades[1], George Lefkaritis[1], Andreas Kourtellaris[1], Nikos Chronakis[1,†]
[1]Dept. of Chemistry, University of Cyprus, Cyprus

A series of catechol-derived propargyl diols were synthesized and submitted to cyclization with malonyl dichloride, under basic conditions, to afford the corresponding 13-membered macrocyclic diesters. Product distribution appeared to be associated with the choice of protecting group for the catechol hydroxy substituents. Diverse protecting groups, able to fine-tune the (stereo)electronic contribution of each substituent to the π-conjugated system were investigated. In the cases of a trifluoromethylsulfonate-substituted or a conformationally-restricted cyclohexyl dioxolane-comprising propargyl diol substrate, as well as the O-substituent-free propargyl diol counterpart, the reaction led to the expected macrocyclization, alongside traces of a 26-membered macrocyclic tetraester, without any indication of a competing hydrochloride addition to a propargyl triple bond. However, upon switching to silyl or methyl groups as catecholic O-atom protecting groups, hydrochloride addition occurred on a triple bond under the cyclization conditions, leading to formation of macrocyclic, vinyl chloride adducts, along with the expected intact 13-membered macrocycle. In either case, no metal catalysis was required, while the reaction was performed at ambient temperature. Control experiments involving alternative conditions and hydrochlorination agents, which may form in situ in the original reaction, were conducted, to provide insight on mechanistic aspects.

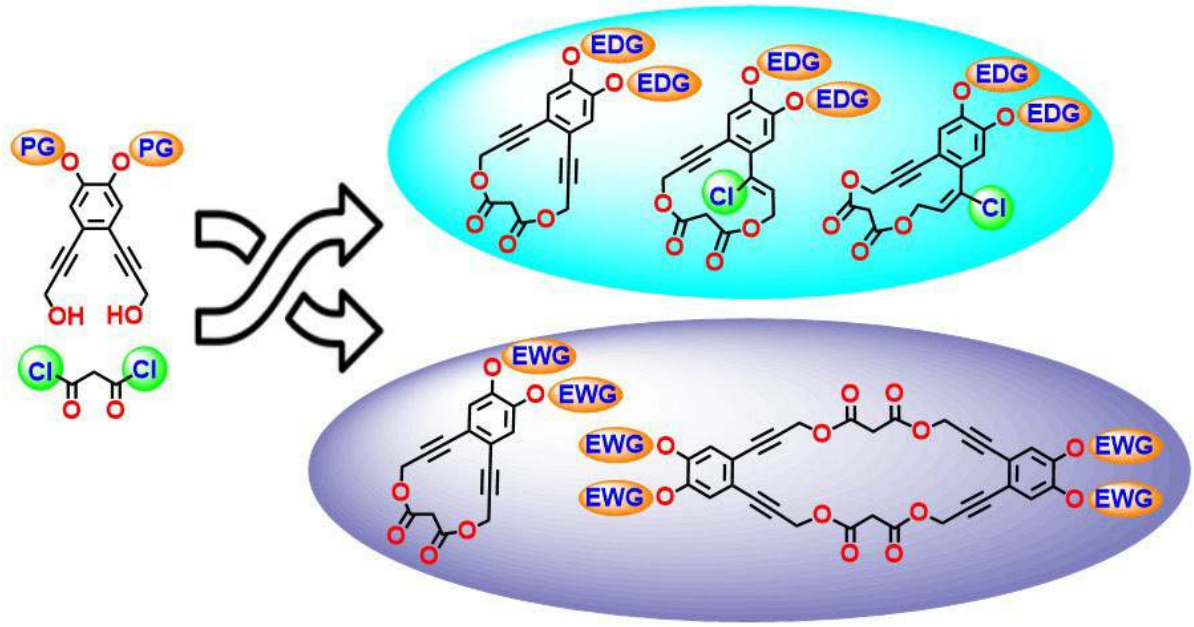


Fig. 1. Macrocyclization of catechol-derived propargyl diols with malonyl dichloride revealed (stereo)electronic effects of hydroxy protecting groups, leading to either 13- and 26-membered macrocycles for EW-PGs or intact and hydrochlorinated macrocycles for ED PGs.

MDR - D4 - P01
Molecular design of acrylic polymers for controlling the damping behavior of epoxy composites

Yong Rok Kwon[1], Jung Soo Kim[1], Sihun Jang[1], Dong Hyun Kim[1], Ju-Hee So[1,*]
[1]korea Institute of Industrial Technology, Republic of Korea

Epoxy-based composites are widely used in semiconductor packaging processes due to their excellent mechanical strength and thermal stability. However, they are susceptible to interfacial delamination and cracking under thermal cycling conditions, where repeated stresses are generated. In particular, for semiconductor post-processing film materials, including die-attach films, the ability to relax stresses arising from the coefficient of thermal expansion mismatch between the chip and the substrate is a critical factor governing long-term reliability.
From this perspective, this study aims to systematically investigate the effects of the glass transition temperature (Tg) and molecular weight (Mw) of acrylic polymers on the damping behavior of epoxy composites. Acrylic polymers with controlled Tg and Mw were synthesized and incorporated into epoxy resins, and the resulting composites were evaluated using dynamic mechanical analysis. The storage modulus, loss modulus, and tan δ responses were analyzed to characterize the viscoelastic behavior of the systems. In particular, the position, width, and area of the tan δ peak were analyzed in detail to evaluate the damping characteristics that are closely related to stress relaxation. Through this approach, this work seeks to identify key acrylic polymer design parameters for achieving the thermal cycling reliability required in semiconductor post-processing films and to provide fundamental insights into structure–property relationships of epoxy-based film materials from a damping perspective.

MDR - D4 - P02

The design & synthesis of fluorescent self-assembled monolayers for optical applications

Ben Clarke[1a], Elisabeth Bancroft[1b], Samuel P Jarvis[1b], Benjamin Robinson[1b], Jonathan S. Ward[1a]
[1a]Chemsitry Dept., Lancaster University, UK;[1b]Physics Dept., Lancaster University, UK

Controlling the orientation of π-conjugated molecules is an important area of research, as molecular orientation plays a critical role in determining the efficiency of optoelectronic devices.[1] However, many high-performance devices are currently fabricated using vacuum evaporation techniques, which are energy intensive and suffer from extremely low material utilisation.[2] Developing alternative, solution-processed routes that enable precise control over molecular orientation therefore represents an attractive and more sustainable strategy.

In this work, we introduce a novel approach towards controlling molecular orientation based on greener, solution-processed methods. The control of tilt angle within self-assembled monolayers (SAMs) is exploited to influence the orientation of π-conjugated molecules at transparent conducting oxide interfaces. A series of carbazole donor–acceptor emitters were designed and synthesised, with particular emphasis placed on achieving the high levels of purity required for reliable self-assembly.

Monolayers were deposited onto indium tin oxide (ITO) substrates, and their formation and organisation were investigated using a combination of X-ray photoelectron spectroscopy (XPS) and other surface characterisation techniques. These techniques reveal high binding efficiencies, and the effects of deposition parameters and post-deposition treatment on film quality and surface coverage was also examined.

Finally, the effect of surface binding and molecular orientation on photophysical behaviour was investigated. Solution-phase studies show bright blue charge-transfer emission with solvatochromic behaviour, while solid-state measurements are ongoing but indicate bright emission. Future work will demonstrate how controlled self-assembly at oxide surfaces can be used to tune optical behaviour, highlighting the potential of SAM-based strategies for the development of efficient, sustainable optoelectronic devices.

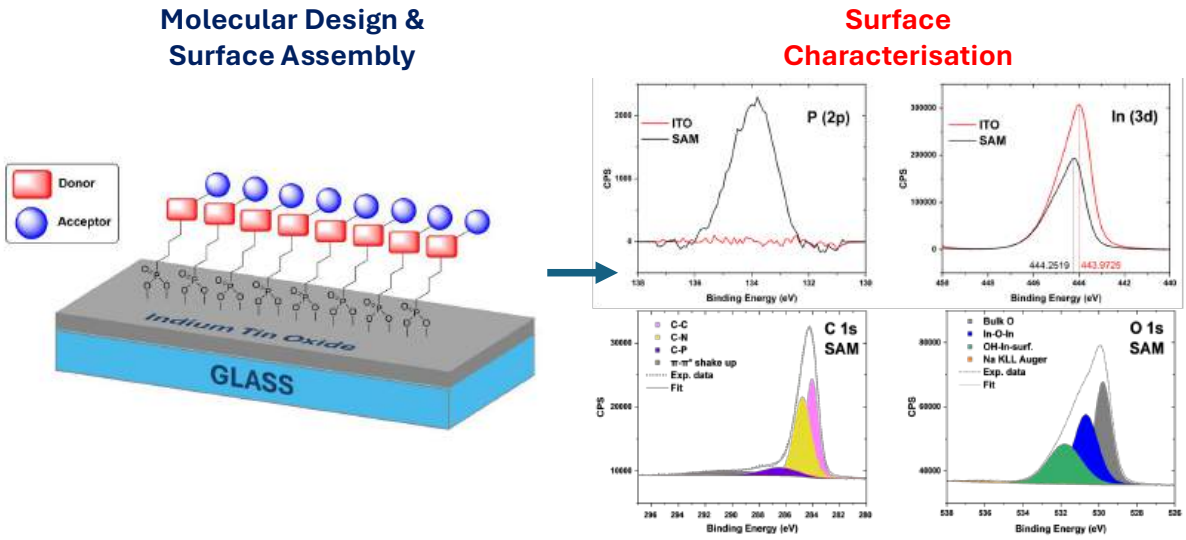


Fig. 1. Left: Schematic representation of donor–acceptor self-assembled monolayers (SAMs) on ITO. Right: XPS spectra confirming SAM binding to the ITO surface.

[1]Schmidt, T. D.; Lampe, T.; R, D. S. M.; Djurovich, P. I.; Thompson, M. E.; Brütting, W., *Phys. Rev. Appl.* **2017**, *8* (3), 037001
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MDR - D4 - P03

Synthesis and evaluation of boronate precursors for stable astatine radiopharmaceuticals

Arne Hendrickx[1], Daniel Torralba Maldonado[1], Maarten Vanermen[2], Sarandeep Kaur[2], Ingrid De Meester[3], Filipe Elvas[2], Hans De Winter[1], Pieter Van Der Veken[1]

[1]Laboratory of Medicinal Chemistry, Faculty of Pharmaceutical, Biomedical and Veterinary Sciences, University of Antwerp, Belgium; [2]Molecular Imaging and Radiology, Faculty of Medicine and Health Sciences, University of Antwerp, Belgium; [3]Laboratory of Medical Biochemistry, Faculty of Pharmaceutical, Biomedical and Veterinary Sciences and Infla-Med Centre of Excellence, University of Antwerp, Belgium

Fibroblast activation protein (FAP) targeting of radionuclides is investigated as a therapeutic strategy in many domains of oncology. UAMC-1110, a potent and highly selective FAP-inhibitor discovered in our group, is widely used as a FAP-targeting vector in clinically developed oncology theranostics.[1,2] One of the underrepresented radionuclides in this effort is ^{211}At. This alpha-emitting radionuclide is of great interest to nuclear medicine due to its ability to induce irreversible cell death in tumors. Introducing it in a metabolically stable form into a radiopharmaceutical, however, is an enduring challenge.[3] A major limitation for *in vivo* applications is de-astatination, a phenomenon where a carbon–astatine bond is cleaved, leading to suboptimal tumor irradiation and off-target accumulation of free astatine in healthy tissue.

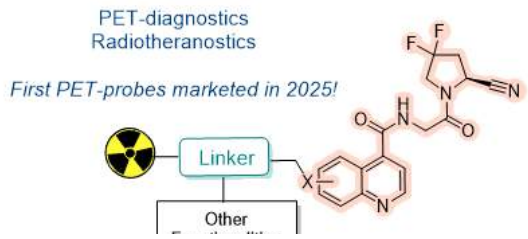

Fig.2. FAP-targeting radiotheranostics

To effectively tackle this problem, we propose innovative astatine-bearing prosthetic groups and that allow chemical stabilization of the C-At bond by modifying the electronic and steric properties.

A first series of boronic precursors has been synthesized for radiolabeling. Boron-based precursors were selected since our group was successful in optimizing astatination yields with this type of compounds. An additional advantage is that boronate cross-coupling chemistry is extremely well documented because of the importance of Suzuki-Miyaura chemistry. The synthesis of these boronic precursors, nonetheless, came with several challenges, which were solved through optimization and application of literature-reported techniques.

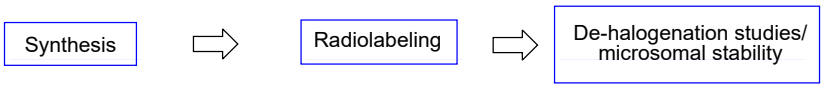

Fig. 3. *De-astatination stability screening cascade*

The resulting fragments were radiolabeled with ^{211}At and screened *in vitro* for their resistance to de-astatination.[4] This experimental effort is backed with Density Functional Theory (DFT)-based bond dissociation energy (BDE) calculations, to find the optimal substitution for C-At bond stability. Ultimately, the goal is to assess optimized stable ^{211}At-FAPi radiotheranostic compounds in preclinical mouse models.

[1]Jansen, K., Heirbaut, L., Verkerk, R., Cheng, J. D., Joossens, J., Cos, P., ... & Van der Veken, P. **2014**, Journal of medicinal chemistry, 57(7), 3053-3074.
[2]Van Rymenant, Y., Tanc, M., Van Elzen, R., Bracke, A., De Wever, O., Augustyns, K., ... & Van Der Veken, P. **2021**. Frontiers in Chemistry, 9, 640566.
[3]Mador, S. D., Yssartier, T., Le Questel, J. Y., Montavon, G., Guérard, F., & Galland, N. **2025**, *ACS Physical Chemistry Au*.
[4]Fouinneteau, R., Maingueneau, C., Galland, N., Perrio, C., & Guérard, F. **2025**. *Scientific Reports*, *15*(1), 16877.

MDR - D4 - P04

Ring-opening polymerization of δ-tetradecalactone for oil-soluble poly(ester) lubricant additives with tunable molecular weight

Hae Chan Kim[1], Sue Been Lee[1,2], Si Hoon Jang[1], Jung Soo Kim[1] Dong Hyun Kim[1]
[1]User Convenience Technology R&D Dept., Korea Institute of Industrial Technology (KITECH),South Korea; [2]Dept. of Materials Science and Chemical Engineering, Hanyang University, South Korea

Cyclic lactones bearing long alkyl substituents represent an effective platform for oil-soluble polymeric lubricant additives due to the coexistence of polar ester functionalities and hydrocarbon-compatible side chains. In this work, δ-tetradecalactone (δ-TDL), a C14-substituted δ-lactone, was investigated as a monomer for the preparation of poly(ester)-based lubricant additives via ring-opening polymerization (ROP). Polymer architectures with controlled molecular weight were achieved by regulating the monomer-to-initiator ratio, enabling the preparation of multiple polymer grades spanning low to high molecular weight regimes. The synthesized polymers were characterized by nuclear magnetic resonance spectroscopy and gel permeation chromatography, confirming monomer conversion, chain structure, and effective molecular weight control with narrow dispersity. Lubricant formulations containing the polymers were prepared by blending into commercial base oils at low treat rates. The viscosity–temperature behavior was evaluated through kinematic viscosity measurements, and viscosity index (VI) enhancement was observed as a function of polymer molecular weight. Low-temperature flow behavior was evaluated by pour point measurements, where a noticeable depression of the pour point was observed in polymer-containing lubricant formulations relative to the neat base oil.
The long alkyl side chain of δ-TDL contributed to excellent oil solubility and compatibility, while the ester backbone provided polar interactions with metallic surfaces, supporting both thickening efficiency and boundary lubrication performance. These results demonstrate that lactone-derived polymeric additives constitute a versatile and tunable design platform for lubricant applications, where molecular weight and polymer architecture play a critical role in determining macroscopic performance.

Acknowledgements: This work was supported by the Technology Innovation Program (Parts and Materials Technology Development) under Grant RS-2024-00433164, funded by the Ministry of Trade, Industry and Energy (MOTIE, Republic of Korea).

MDR - D4 - P05

Epoxy-terminated polyurethanes as effective toughening agents for epoxy molding compounds

Sue Been Lee[1,2], Hae Chan Kim[1], Si Hun Jang[1], Jung Soo Kim[1], and Dong Hyun Kim[1,*]

[1]Korea Institute of Industrial Technology, Republic of Korea; [2]Hanyang University, Republic of Korea

A toughening agent is an additive incorporated into epoxy resins to absorb and dissipate applied stress, thereby improving the material's toughness. Although epoxy resins exhibit excellent mechanical and thermal properties, their inherent brittleness limits practical applications. Therefore, epoxy-terminated polyurethanes (EPUs) were employed as toughening agents to overcome this drawback.

EPUs were synthesized via bulk polymerization of isophorone diisocyanate and polyols, followed by the introduction of glycidol for epoxy end-functionalization of the polymer chains. Three different polyols, polyethylene glycol, polypropylene glycol (PPG), and polytetrahydrofuran, were employed as variables to investigate the properties of the EPUs. The synthesized EPUs were characterized by Fourier transform infrared spectroscopy, which confirmed urethane linkage and the introduction of epoxy functional groups. The mechanical properties and viscoelastic behavior were evaluated using tensile testing and dynamic mechanical analysis. Thermal properties were analyzed by differential scanning calorimetry and thermogravimetric analysis. Furthermore, scanning electron microscopy was utilized to examine fracture morphologies, providing insight into the toughening mechanism. The PPG-based EPU exhibited the highest enhancement in toughness of epoxy resins, as revealed by a comparative evaluation of EPUs prepared with different polyols. Based on these toughening effects, EPUs are expected to serve as effective toughening agents for epoxy systems requiring improved toughness, such as epoxy molding compounds.

MDR - D4 - P06

Toughening effect of core-shell impact modifiers on epoxy resin maintaining thermal stability

Sun Ho Seok[1,2], Min Jin Seong[1,2], Jun Ho Park[1], Jung Soo Kim[1], Sihun Jang[1], Hwa Sung Lee[2] and Dong Hyun Kim[1,*]

[1]Korea Institute of Industrial Technology, Republic of Korea; [2]Hanyang University, Republic of Korea

Impact modifiers are widely used to enhance the toughness of thermosetting polymer resins, including epoxy (EP), by improving energy dissipation and crack resistance. Among them, liquid rubbers enhance the toughness of EP. However, their incomplete phase separation reduces thermal stability of EP, such as glass transition temperature (T_g). Therefore, core-shell impact modifiers (CSIMs) have been studied to improve the toughness of EP while maintaining thermal stability. Two types of CSIMs were synthesized via semi-batch emulsion polymerization: non-reactive CSIM and reactive CSIM. Both CSIMs use butyl acrylate as the core monomer. The core was synthesized by seed emulsion polymerization, then the shell was synthesized on the surface of the core via semi-batch emulsion polymerization. For the shell, non-reactive CSIM used methyl methacrylate (MMA), while reactive CSIM used a copolymer of MMA and glycidyl methacrylate (GMA). The reason why GMA is applied in reactive CSIM is that its epoxy functional groups provide high compatibility with EP resin and react with the curing agent. The core-shell structure of CSIMs was characterized by using transmisiion electron microscopy. The thermal properties of CSIM applied EP were evaluated using differential scanning calorimetry and thermogravimetric analysis, while their mechanical properties were examined through impact and flexural test. The impact and flexural strength of EP with reactive CSIM have improved without a significant decrease in T_g compared to neat EP and EP with non-reactive CSIM, which is attributed to the epoxy groups of GMA present in the shell participating in the curing reaction of EP resin, enhancing the cross-linking density. The dispersibility of the CSIM was verified by observing the fracture surface of the composites under scanning electron microscopy.

MDR - D4 - P07
Theoretical design principles for spin-selective relaxation in photoexcited metal complexes

Yuki Yamamoto[1], Yuki Kurashige[1,2,3]
[1]Dept. of Chemistry, Graduate School of Science, Kyoto University, Japan; [2]JST-CREST; [3]JST-FOREST

Electron spin polarization in molecular systems is a phenomena where the non-Boltzmann population distribution among spin sublevels of electronic states with spin multiplicity greater than two. In recent years, it has attracted considerable attention from the perspective of quantum control technologies, such as optically detected magnetic resonance (ODMR) and dynamic nuclear polarization (DNP). Although various mechanisms for generating electron spin polarization have been proposed—some still at the hypothesis stage—one relatively reliable mechanism is spin-selective intersystem crossing (SS-ISC). In the SS-ISC mechanism, for example, photoexcitation of pentacene generates an excited singlet (S1) state, and during intersystem crossing to a nearby excited triplet (T2) state, differences in transition rates to the three spin sublevels T2(X), T2(Y), and T2(Z) produce spin polarization in T1. These differences in transition rates are considered to originate from the anisotropy of spin–orbit coupling (SOC), which mediates the spin-forbidden intersystem crossing process.
In this study, we theoretically predict photoinduced spin polarization in metal complexes with triplet ground states. Three complexes—Cr(o-tolyl)$_4$ (1-Cr), $(C_6F_5)_3$trenVCNtBu (2-V), and $^{Me}Tp_2Ni$ (3-Ni)—were investigated. The energies of low-lying excited states, spin–orbit coupling matrix elements between relevant states, and zero-field splitting (ZFS) parameters necessary for predicting spin polarization were calculated using multireference electronic structure theory, namely the complete active space self-consistent field (CASSCF) method and second-order perturbation theory on top of the CASSCF (CASPT2). In addition, the spin selectivity of intersystem crossing was analyzed from a group-theoretical perspective including molecular vibrational modes, and the results were compared with the calculated SOC matrix elements.
The calculated ZFS parameters for all complexes were sufficiently small to allow microwave manipulation. For 1-Cr and 2-V, excited singlet states were found to lie below the lowest excited triplet state, and the anisotropy of the SOC matrix elements suggests that spin-selective intersystem crossing can occur. Furthermore, we theoretically investigated the spin selectivity of relaxation processes from singlet states to the triplet ground state, incorporating vibronic coupling effects. Finally, we propose molecular design strategies to enhance spin selectivity beyond that achievable through vibronic interactions alone.

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MDR - D4 - P08
Improving the toughness of electronic adhesives through epoxy-acrylic hybridization

Min Jin Seong[1,2], Sun Ho Seok[1,2], Jung Soo Kim[1], Yong Rok Kwon[1], Dong Hyun Kim[1], Tae Hyun kim[2] and Ju-Hee So[1,*]
[1]Korea Institute of Industrial Technology, Republic of Korea; [2]Hanyang University, Republic of Korea

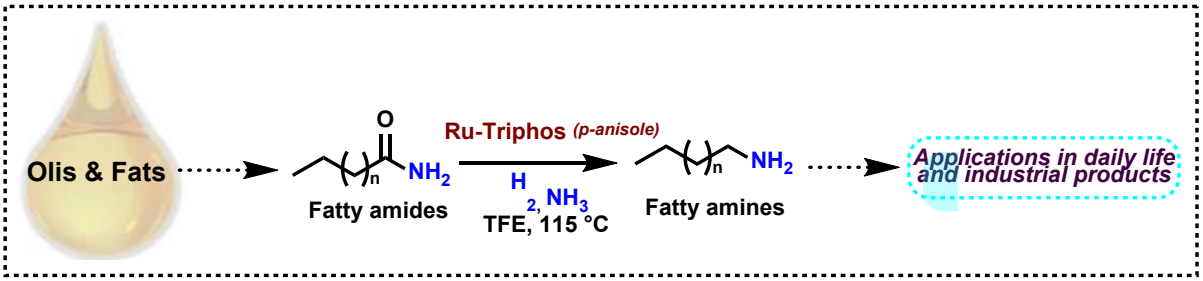
Epoxy resin is a representative thermosetting polymer that is widely used for electronic and semiconductor adhesives, high-reliability structural adhesives, surface coatings, paints, protective layers, owing to its excellent adhesion, high mechanical strength, outstanding chemical and corrosion resistance, and good electrical properties. However, the high crosslink density of epoxy resins can embrittle the material, thereby reducing resistance to crack initiation and propagation. In particular, in structural and electronic adhesive applications where interfacial stress concentration occurs, such brittleness can lead to fracture or delamination, which is a major factor limiting the application of epoxy resins. To overcome these limitations, acrylic rubber with a saturated backbone and various pendant groups has been widely used as a toughness modifier for epoxy resins. In this study, acrylic rubbers with varying epoxy-group content were synthesized by controlling the glycidyl methacrylate (GMA) content, and adhesive films were prepared by blending the acrylic rubbers with an epoxy resin and a curing agent. The acrylic rubbers were synthesized using butyl acrylate (BA), 2-hydroxyethyl acrylate (HEA), methyl methacrylate (MMA), and GMA as monomers. BA and MMA were used to tailor the flexibility and stiffness of the acrylic rubber, and HEA was introduced to enhance adhesion to substrates through hydroxyl groups. GMA is an epoxy-functional monomer that enables the formation of chemical bonds with the epoxy matrix and can enhance compatibility. The effects of epoxy-group content on the toughness and thermomechanical properties of the epoxy/acrylic-rubber adhesive films were systematically evaluated. The toughness and adhesion strength of the adhesive films were evaluated using tensile and T-peel tests. Furthermore, the thermal and viscoelastic behaviors of the adhesive films were analyzed using differential scanning calorimetry and dynamic mechanical analysis.

MDR - D4 - P09

General and selective ruthenium-catalyzed hydrogenation of primary amides to primary amines under mild conditions

Vishakha Goyal[1,2], Chakreshwara Kuloor[1], Radek Zbořil[2,3], Mathias Beller[1], Rajenahally V. Jagadeesh[1,2]
[1]Leibniz Institute for Catalysis. e.V., Germany; [2]Nanotechnology Centre, Centre for Energy and Environmental Technologies, VSB-Technical University of Ostrava, Czech Republic; [3]Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute, Palacký University Olomouc, Czech Republic

Catalytic hydrogenations are an essential class of synthetic processes, which are widely used in both research laboratories and industries to produce fine and bulk chemicals as well as pharmaceuticals, and agrochemicals.[1,2] Hydrogenation of amides continues to be one of the most difficult reductive transformations in organic synthesis.[3,4] Despite significant efforts in past decades, there is no general protocol reported allowing the synthesis of various primary amines from the corresponding primary amides using molecular hydrogen. To perform this challenging reaction, here we report a specific homogeneous ruthenium catalyst based on the methoxy-substituted triphos ligand (Triphos(p-anisole)). In the presence of this Ru-catalyst system, industrially relevant, functionalized, and structurally diverse aromatic, heterocyclic and aliphatic primary amides including fatty amides were selectively hydrogenated to produce the corresponding primary amines under comparably mild conditions (typically 115 °C and 10 bar H_2). The resulting amines are valuable compounds with diverse applications in chemistry, medicine and biology as well as in materials and energy technologies.



Acknowledgements: We thank the German Research Foundation (DFG project numbers 670389-NFDI2/1 and 447724917), and the State of Mecklenburg-Vorpommern for financial and general support. We gratefully acknowledge the financial support from the European Union under the REFRESH-Research Excellence or Region Sustainability and High-tech Industries project number CZ.10.03.01/00/22_003/0000048 via the Operational Programme Just Transition. Vishakha Goyal acknowledges the financial support of the European Union under the “MSCA Fellowships CZ at VSB-TUO 2.0” project, reg. nr. CZ.02.01.01/00/22_010/0008714 within the Johannes Amos Comenius Operational Programme. We are thankful to the analytical team of the Leibniz-Institut für Katalyse e.V. for their excellent service.

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MDR - D4 - P10

Structure activity relationship directed development of an internal standard for an electrochemical fentanyl detector

Sean Betteridge[1], Tristan Ruigrok[2], Dan Bizzotto[3], Glenn Sammis[4]
University of British Columbia, Canada

Between 2016 and 2023, Canada experienced 44,592 opioid-related deaths, making opioids the leading cause of accidental death among Canadians under 65.[1,2] Despite their addictive potential, opioids remain essential for pain management, palliative care, and end-of-life care.[3,4] Since 2013, the prevalence of fentanyl and other potent synthetic opioids has accelerated overdose rates.[5] Fentanyl, with a potency 100–200 times greater than morphine,[6] accounted for 83% of opioid overdose deaths in Canada in 2023.[1]

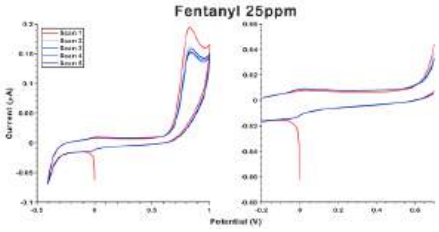

Figure 1: Fentanyl CV

To address the need for rapid fentanyl detection, this work develops a point-of-use electrochemical detector for fentanyl quantification in biological fluids and illicit drug samples. Detecting trace fentanyl in illicit substances can enhance harm-reduction efforts by improving drug testing reliability. Key features include high-throughput screening (<5 min analysis time with concurrent processing), ease of use, compact design, cost efficiency, and a detection threshold exceeding current field-deployable methods.

A key challenge is the lack of a suitable internal standard with electrochemical behavior comparable to fentanyl. To address this, novel fentanyl analogues were synthesized with targeted structural modifications to tune redox potentials while reducing opioid potency. Over 50 analogues were prepared, identifying three candidates with redox signals offset by approximately ±0.3 V from fentanyl's signal at 0.08 V. Ongoing work includes evaluation in mixed drug samples, and studies in biologically relevant matrices.

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MDR - D4 - P11

Monomer structure and feed protocol effects on microstructure and processing of resorcinol based polyarylates

Ayşe Zeyneb Erten[1,2], A. Ersin Acar[1]*

[1]Dept. of Chemistry, Boğaziçi University, Istanbul, Türkiye; [2]CFN Kimya Sanayi ve Dış Ticaret A.Ş., Kocaeli, Türkiye

Resorcinol based polyarylates intrinsically absorb UV radiation through aromatic arylate chromophores, enabling built in UV screening. Under UV exposure, arylate linkages can undergo a photo-Fries rearrangement to form o-hydroxybenzophenone derivatives that may contribute to sustained UV absorption during ageing. Beyond overall composition, the sequence distribution established during solution polycondensation can influence segmental heterogeneity, glass transition temperature characteristics, and solution processing behaviour. Here, we evaluate how aliphatic diol architecture and monomer addition order jointly control microstructure and properties in resorcinol based polyarylates.

Polyarylates were synthesized from aromatic diacid chlorides and resorcinol together with one of two aliphatic diols providing contrasting conformational rigidity: a cyclic (stiff) diol and a linear (flexible) diol. For each aliphatic diol, three feed protocols were applied at identical target stoichiometry: (i) one pot polymerization using a premixed diol blend, (ii) sequential addition with resorcinol introduced first, and (iii) sequential addition with the aliphatic diol introduced first. We hypothesize that differences in relative diol reactivity during early oligomer formation generate protocol dependent sequence distributions, while monomer architecture sets the baseline chain stiffness.

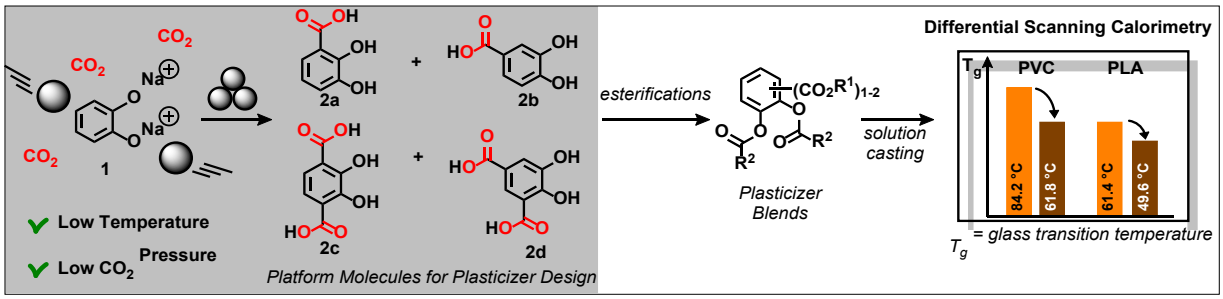
The resulting polymers were comprehensively characterized by NMR, FTIR, UV-Vis, GPC, DSC to correlate molecular architecture with thermal transitions. Standardized solubility and precipitation tests were used to compare aggregation and isolation behaviour. The study demonstrates that varying the feed protocol allows for tuning of segmental blocks, which directly modulates solution processability and solvent polymer interactions without compromising the intrinsic UV absorbing character. By controlling the sequence distribution, we report a route to engineer polyarylates with tailored solubility profiles, offering a advantage for specialized coating applications and thin film processing.

MDR - D4 - P12

A mechanochemical Kolbe-Schmitt reaction: Catechol carboxylation provides building blocks for renewable plasticizers

Dries De Vos[1], Victoria S. Pfennig[2], Arno Goddé[1], Robby Vroemans[1], Tobias Krückel[2], Nicole Marcinkowska[2], Ettore Bartalucci[2,3], Thomas Wiegand[2,3], Carsten Bolm[2], Bert U. W. Maes[1]
[1]Dept. of Chemistry, UAntwerp, Belgium; [2]Dept. of Chemistry, RWTH Aachen University, Germany; [3]MPI for Chemical Energy Conversion, Germany

Catechol, produced annually at 40 ktons, is a key commodity chemical prepared from phenol derived from crude oil.[1] Recently, it has been derived from non-edible biomass in biorefineries, offering a renewable alternative to fossil carbon for chemical production.[2-6] An interesting transformation is its carboxylation with the greenhouse gas CO_2 as a C1-reactant, thereby allowing to generate dihydroxybenzoic acids with 100% renewable carbon featuring handles for further derivatization. However, the classical Kolbe-Schmitt reaction of disodium catecholate (**1**) with CO_2 requires harsh reaction conditions involving high temperature (up to 225 °C) and CO_2 pressures (up to 76 bar).[7-8] In this work, disodium catecholate (**1**) was carboxylated by mechanochemical Kolbe-Schmitt reaction with CO_2, providing a mixture of mono- and dicarboxylated catechol derivatives (**2a**-**2d**) at room temperature under low CO_2 pressure (4 bar).[9]
From the individual catechol-based mono- and dicarboxylic acid reaction products, a library of renewable plasticizers was synthesized through esterification of the carboxylic acid and the phenolic hydroxy groups. The resulting esters were evaluated as plastic additives in poly(vinylchloride) (PVC) and poly(lactic acid) (PLA), revealing plasticizing efficiencies competitive to commercial plasticizers.[9] The best performing substitution pattern was also effective when applied to the ball mill-derived mixture of mono- and dicarboxylated catechols, eliminating the need for resource-intensive (chromatographic) separation.



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MDR - D4 - P13

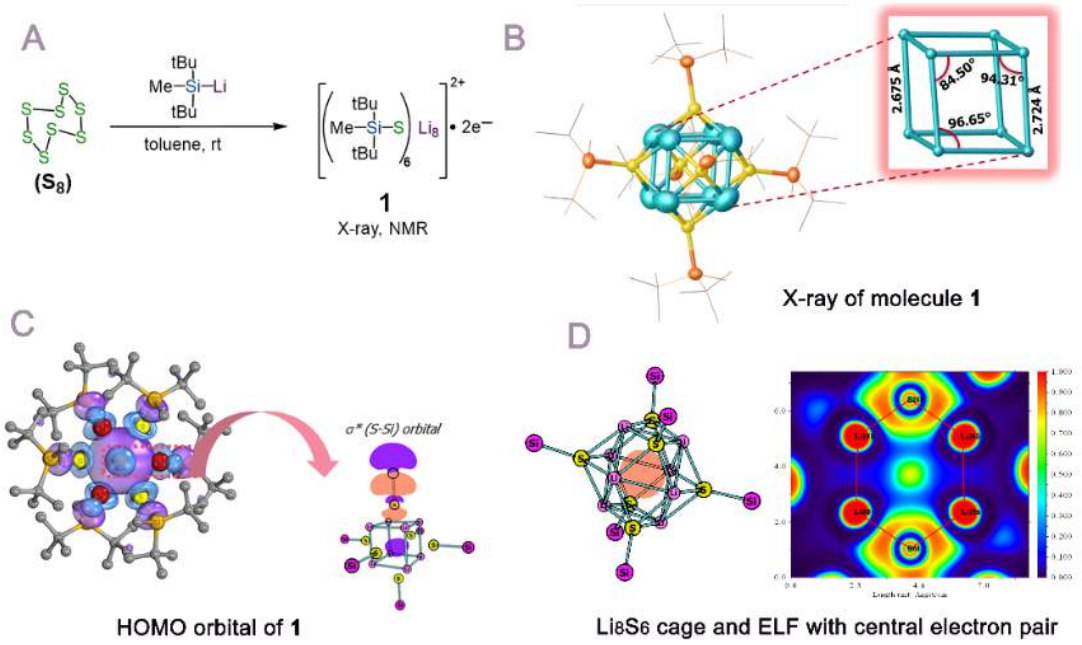
Two electrons in a Li-S C-cage: A novel lithium cubic electride - $[(tBu_2MeSiS)_6Li_8]^{2+}•2e^-$

Devendra Yadav[1,2], Alexander Kaushansky[1], Yuri Glagovsky[1], Dmitry Bravo-Zhivotovskii[1,2], Malachi Noked[2]*, Yitzhak Apeloig[1]*

[1]Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Israel; [2]Institute of Nanotechnology and Advanced Materials, Bar Ilan University, Israel

Electrides - materials in which electrons serve as anions, are of fundamental importance for catalysis, energy storage, and quantum materials owing to their exceptional electron-donor properties.[1-2] However, despite extensive progress in solid-state systems, the realization of thermally stable, single-molecule electrides with centrally stored electrons has remained a major synthetic challenge. In 2003, Matsuishi *et al.* reported the first thermally stable electride $[Ca_{24}Al_{24}O_{64}]^{4+}•4e^-$, formed by removing central O^{2-} ions from extended oxide cages, thereby enabling electron confinement within the nanoporous framework.[3] While such solid-state electride materials are well studied, singly isolated electrides with high thermal stability and truly central electron(s) remain mostly unknown.

Here we report an unprecedented lithium–sulfur–silyl cluster, $[(tBu_2MeSiS)_6Li_8]^{2+}•2e^-$, (**1**) - the **first thermally stable and structurally characterized molecular electrides featuring confined interstitial electrons** (Scheme 1, A-B). X-ray and ELF analyses confirm the confinement of an interstitial electron pair within the S_6Li_8 cluster (Scheme 1, D) and the cubic Li_8 cavity of 15.23 Å^3. NBO data reveal dominant contributions from Li(ry) and σ*(S–Si) orbitals (Scheme 1C). The electride-like HOMO is high-lying (–1.66 eV) and the HOMO–LUMO gap is small (1.17 eV), indicating strong central electron localization. To the best of our knowledge, **no electrides with high electron density inside a single-isolated molecule cage have been previously reported.** Our findings establish a molecular design paradigm where cavity volume, ligand architecture, and orbital diffuseness can be tuned to access structurally stable, solution-processable molecular electrides.



Scheme 1. (A) Synthesis of **1**; (B) X-ray structure of **1**, showing a Li_8 cubic arrangement; (C) HOMO orbital of **1**, showing σ* (S-Si) orbital contribution; (D) Electron Localized Function (ELF) graph of the Li_8S_6 cage showing the central electron pair density.

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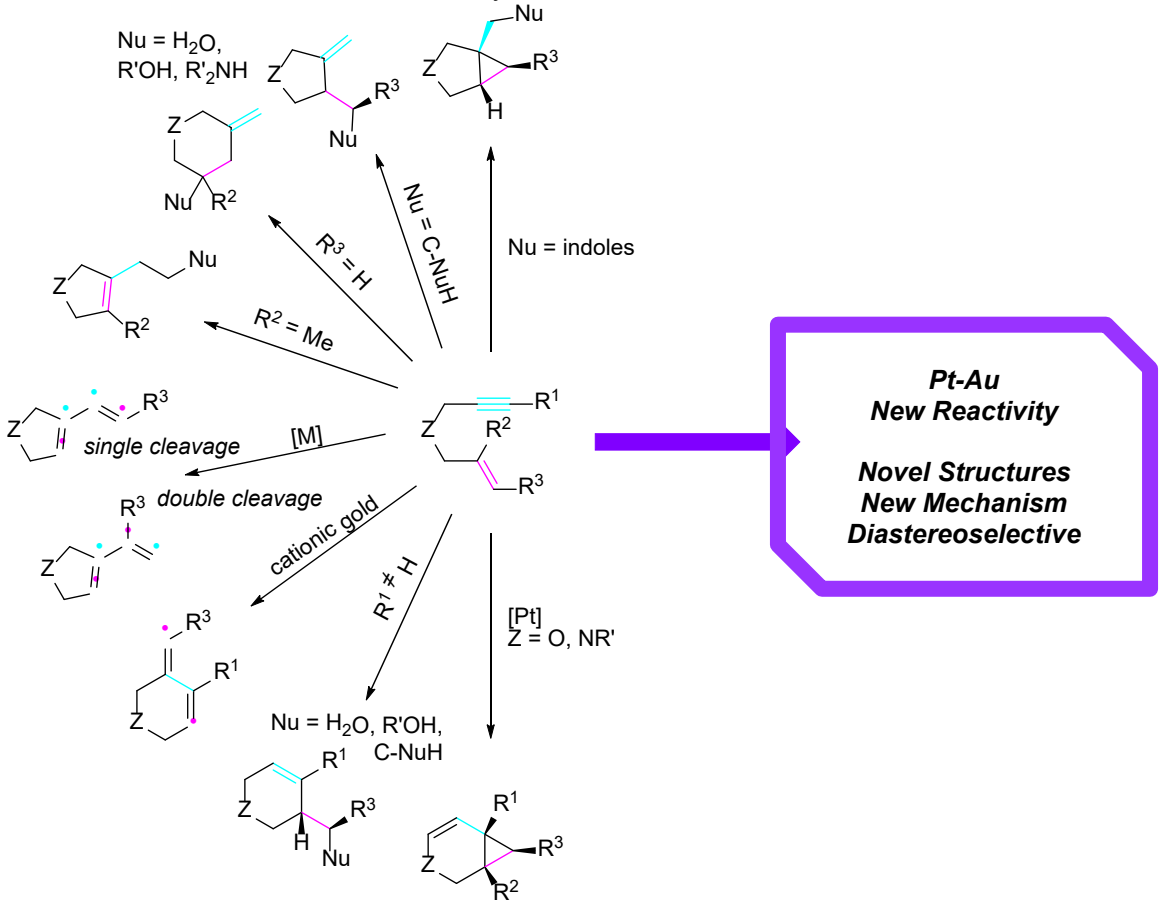
MDR - D4 - P14
Expanding drug-relevant chemical space through Pt-Au bimetallic catalysis

Khaleel Zareen, María Paz Muñoz-Herranz
Lancaster University, UK

Bimetallic catalysis has evolved in recent years as a powerful strategy towards the synthesis of new structures, inaccessible through monometallic systems. Homogeneous Pt-Au bimetallic catalysis has scarcely been reported on, except for by Muñoz and co-workers,[1,2] to achieve novel, azole-containing compounds with promising antimicrobial activity.[3] The key to the enhanced and divergent reactivity established here is due to the highly electrophilic bimetallic carbene intermediate,[4] and, thus, applying this new methodology to known systems that proceed via a gold carbene intermediate should unlock new possibilities. 1,6-Enynes have been known to undergo several different reactions, including the nucleophilic addition of indoles.[5-7] Under Pt-Au bimetallic catalysis, new interactions with 1,6-enynes have been discovered to give divergent reactivity to access new structures diastereoselectively.



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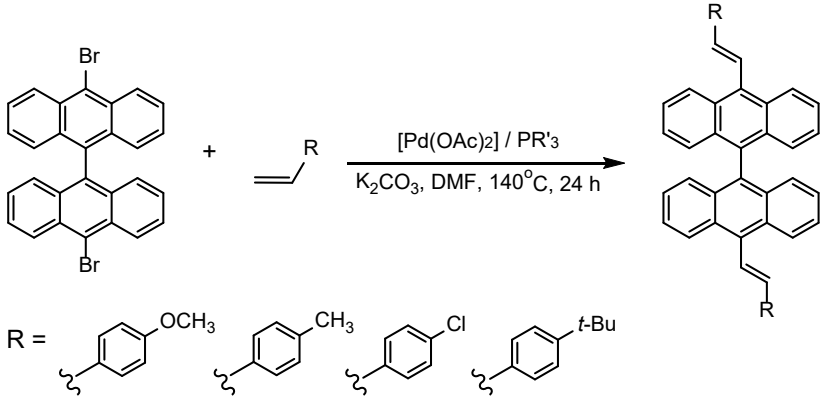
MDR - D4 - P16

Heck coupling of 10,10'-dibromo-9,9'-bianthracene with para-substituted styrenes

Anna Chojnacka[1], Szymon Rogalski[1], Agnieszka Czapik[1], Cezary Pietraszuk[1]
[1]Adam Mickiewicz University,Poznań, Faculty of Chemistry, Uniwersytetu, Poland

Anthracene and bianthracene derivatives play a key role in modern materials chemistry due to their unique photophysical properties, which make them suitable for applications in organic light-emitting diodes (OLEDs)[1] and organic field-effect transistors (OFETs)[2]. One of the most important methods enabling their functionalization is the Heck coupling reaction[3], which is widely used in both organic synthesis and materials chemistry, for example in the preparation of monomers for electronic layers[4].
The aim of this study was to develop a highly selective and efficient procedure for the synthesis of targeted polyunsaturated compounds. Our attention was focused on catalytic systems based on palladium complexes in the presence of Buchwald phosphine ligands and on the investigating the of coupling reactions of 10,10′-dibromo-9,9′-bianthracene with para-substituted styrenes (Scheme 1)[5].



Scheme 1. Synthesis of 10,10'-bis(E-styryl)-9,9'-bianthracenes.

The obtained products were isolated and characterized using ^{1}H and ^{13}C NMR spectroscopy as well as mass spectrometry. For selected compounds, crystal structures were additionally determined. The results clearly confirm that the Heck coupling reaction constitutes an effective and versatile tool for the synthesis of unsaturated 9,9′-bianthracene derivatives with promising luminescent properties, suitable for applications in modern organic electronics.

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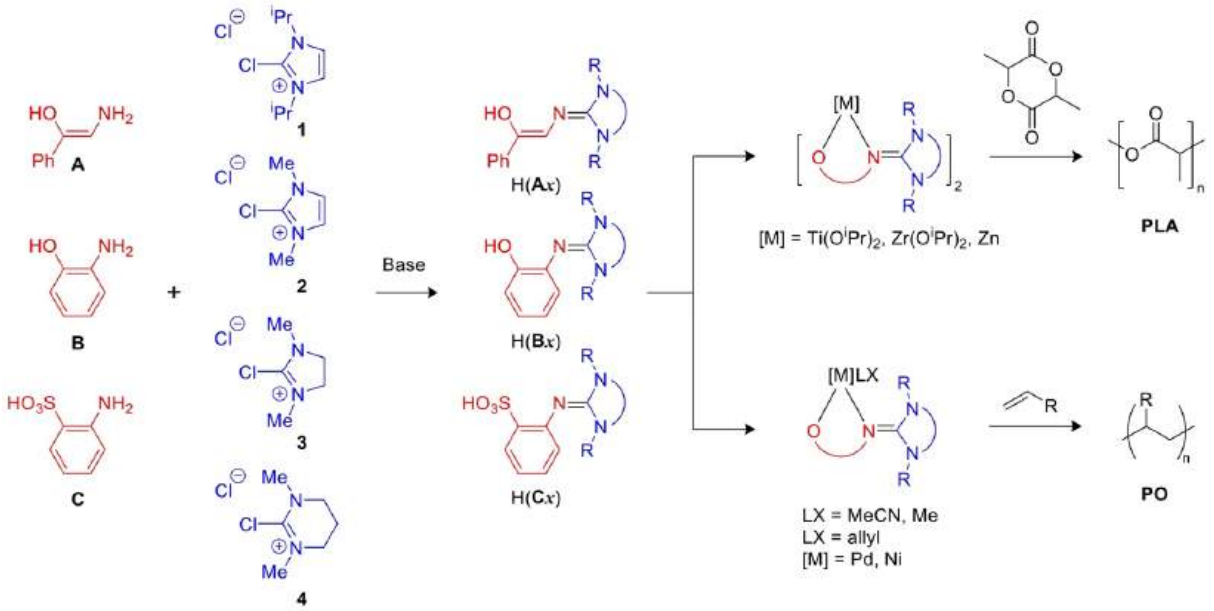
MDR - D4 - P17

Polymerizations using transition metal complexes of monoanionic bidentate guanidine-ethenolate, phenolate and benzene sulfonate ligands

Gino G. Lavoie[1], Víctor Flores-Romero[1], Nicholas L. Miceli[1], Jesse J. LeBlanc[1], Lya E. Campos-Rivera
[1]*York University, Canada*

Modular guanidine-containing ligand platforms have been developed as versatile tools for controlling polymerization catalysis across multiple metal classes (see Scheme). Variations of ligand substituents enable systematic tuning of steric and electronic properties at the metal center, providing direct control over catalyst structure and, in turn, polymer microstructure and physical properties. These ligands support the ring-opening polymerization of lactide using group 12 metals, offering non-toxic alternatives to the tin-based catalysts currently employed industrially and advancing the sustainable production of biodegradable polylactide. Beyond lactide, the same ligand framework can be translated to group 4 and group 10 metals for olefin polymerization, including the challenging copolymerization of non-polar olefins with polar comonomers. This strategy establishes a unified platform for polymer synthesis, in which catalyst reactivity, selectivity, and functional group tolerance can be rationally tailored through ligand design, enabling access to both renewable polyesters and functionalized polyolefins from a common molecular toolbox.



Scheme. Guanidine-containing ligand scaffolds for the synthesis of complexes used in the polymerization of lactide and olefins.

MDR - D4 - P18

Photoinduced radical cascade for the synthesis of enantiopure 2-benzofuranyl *C*-glycosides

Patrícia I.C. Godinho[1,2], Paula Pérez-Ramos[2], Raquel G. Soengas[2], Artur M.S. Silva[1]
[1]LAQV-REQUIMTE, Dept. of Chemistry, University of Aveiro, Portugal; [2]Depto de Química Orgánica e Inorgánica, Universidad de Oviedo, Spain

Benzofurans have gained attention from chemists and biologists over the years, due to their natural occurrence in plants and wide range of biological activities such as anticancer, antiviral, antifungal, anti-inflammatory, antioxidant and so many others. Because of these properties, several synthetic strategies have been developed to synthetize benzofuran derivatives.[1,2] However, despite the importance of glycosylation to improve the the efficacy and pharmacokinetics of drugs, there are limited examples in the literature of the synthesis of *C*-glycosyl benzofuran,[3] so the discovery of new synthetic methods is of great interest.

Herein we report a mild and broadly applicable method for the construction of complex enantiopure *C*-glycosyl benzofuran derivatives through a divergent photoinduced radical cyclization cascade mechanism. Upon irradiation with visible light, spironitrochromenes **1** initiate a radical ring opening to the corresponding nitrodienes **2**, which upon radical denitrative cyclization in the presence of base, affords (1-benzofuran-2-yl)-3-deoxy-α-D-*gluco*-hex-3-enfuranoses **3**. In the absence of a base, the radical denitrative cyclization is followed by a Korblum-type oxidation to finally yield (1-benzofuran-2-yl)-3-deoxy-4-hydroxy-α-D-glucofuranoses **4**.

To sum up, this divergent approach enables the synthesis of a range of enantiopure *C*-glycosyl benzofurans that would otherwise be difficult to prepare.

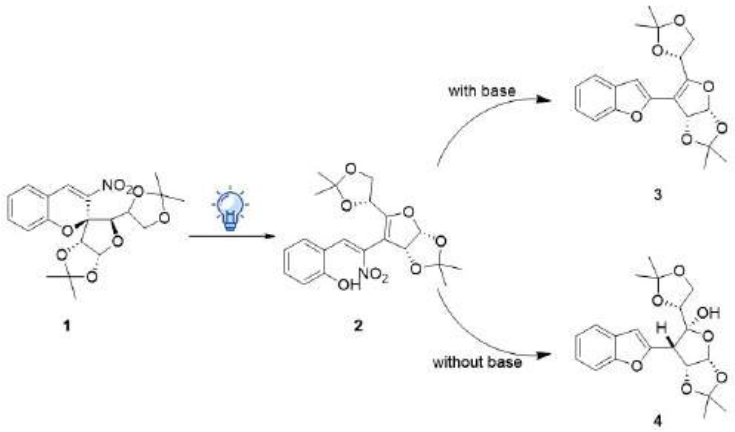


Fig. 1. Synthesis of a range of enantiopure *C*-glycosyl benzofurans.

Acknowledgements: This work received financial support from FCT/MCTES (LAQV-REQUIMTE UID/50006/2025 DOI 10.54499/UID/50006/2025), MCI (PID2022-137893OB-I00), Principado de Asturias (SEK-25-GRU-GIC-24-054), and the EU (European Regional Development Fund-ERDF). Thanks are due to the National NMR Network (PT NMR) partially supported by Infrastructure Project No. 022161 (co-financed by FEDER through COMPETE 2020, POCI and PORL and FCT through PIDDAC).

Funding: Patrícia I. C. Godinho thanks FCT for her PhD grant (2022.11294.BD) and P. P. R thanks University of Oviedo for a predoctoral contract (Proyecto PRP-UO-PUB-ASV-2024TESIS-23).

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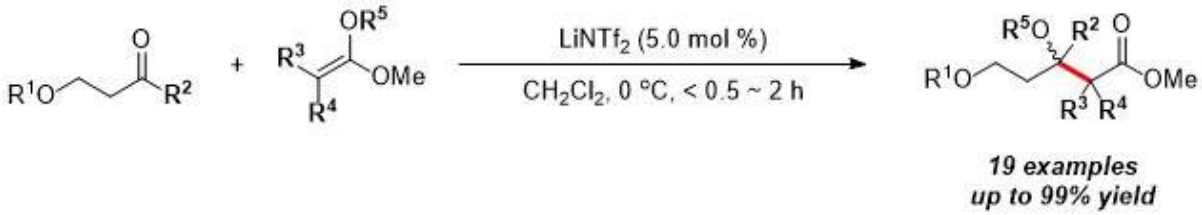
[3]Cao, Z., Zhou, X., Zhang, F., & Zhao, Y. J. Carbohydr. Chem., **2023**, *42*(4–6), 135–157.

MDR - D4 - P19
Synthesis of mevalonate derivatives via LiNTf2 catalyzed Mukaiyama Aldol reaction

Jieun Park[1], Sujin Ahn[1], Eunae Kim[1]
[1]Korea Research Institute of Chemical Technology, South Korea

Mevalonate pathway is a critical metabolic pathway which plays a role in multiple cellular processes by synthesizing isoprenoids, such as cholesterol, vitamin K, coenzyme Q10, and steroid hormones. The substrate of mevalonate has been obtained previously through an aldol reaction of 4-hydroxy-2-butanone with benzyl acetate using LDA, which is unstable, hard to handle, and hazardous to an explosion. As an alternative, we developed a new synthetic method for the preparation of mevalonate derivatives with LiNTf2 as a catalyst of Mukaiyama aldol reaction under the mild condition. LiNTf2 is a safe, cost economy, commercially available, and efficient Lewis acid catalyst. This method is applicable to the reaction of various aliphatic substituted ketone substrates that are challenged and less reactive than aldehydes. This synthetic method has been successfully providing a wide range of tertiary β-siloxy esters with good functional group tolerance. Based on the developed method, we would like to obtain the biologically active new compounds.



This work was supported by the Korea Research Institute of Chemical Technology (IIT25-15) and by the Korea Foundation for Women in Science, Engineering and Technology (WISET 2023-033, WISET 2024-028).

[1]H. Huang, T. Zhang, J. Sun *Angew. Chem. Int. Ed.* **2021**, *60*, 2668-2673.
[2]T. Zhang, Z. Yang, D. Zhou, F. Meng, Z. Han, H. Huang *Org. Biomol. Chem*. **2021**, *19*, 9163–6166.

MDR - D4 - P20
Mild radical construction of tricyclic tetrazoles via in situ diazotization

Garyeong Lee, Chang-Woo Cho*
Dept. of Chemistry, Kyungpook National University, Republic of Korea

Tricyclic tetrazoles are valuable heterocyclic scaffolds with significant potential in medicinal chemistry, yet efficient synthetic approaches to these frameworks remain limited. In particular, 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines have not been previously reported despite their potential bioactivity. Herein, we report a mild and efficient one-pot strategy for the synthesis of tricyclic tetrazoles via cascade diazotization and intramolecular radical C–H heteroarylation of arenes (Figure 1). Readily accessible 1-benzyloxy-5-aminotetrazoles and 1-phenethyl-5-aminotetrazoles were employed as substrates, and the reactions were conducted using sodium nitrite and acetic acid under weakly acidic conditions at room temperature. This protocol proceeds without the need for heating, catalysts, irradiation, or electrolysis, highlighting its operational simplicity. The in situ generated diazonium intermediate undergoes subsequent intramolecular radical C–H heteroarylation to afford tricyclic tetrazole products in good yields (up to 94%) without isolation of intermediates. This method enables the efficient synthesis of previously unexplored 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines as well as 5,6-dihydrotetrazolo[5,1-*a*]isoquinolines. Furthermore, bromo-substituted products were successfully diversified via Suzuki and Sonogashira cross-coupling reactions, demonstrating their synthetic utility. This study provides a straightforward and practical approach to structurally complex tetrazole-fused polycycles under mild conditions, offering new opportunities for the development of bioactive molecules.[1]

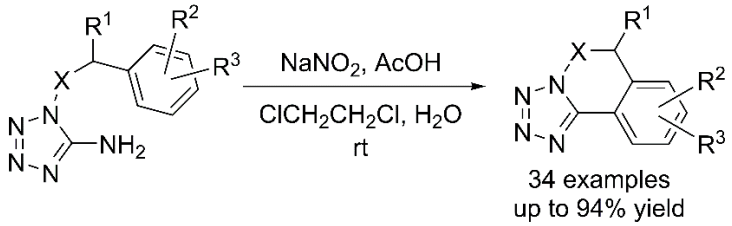


Fig. 1. Cascade diazotization/intramolecular radical C–H heteroarylation of arenes

[1]Ha, H.-J.; Kim, B.; Jo, S.; Kim, S.; Park, J.; Cho, C.-W. *J. Org. Chem.* **2023**, *88*, 2714–2725.

MDR - D4 - P21

Nazarov cyclization of α-SCF_3 Vinyl (Hetero)aryl ketones enabled by trifluoromethylthio group

Ha Yun Nam, Chang-Woo Cho*
Dept. of Chemistry, Kyungpook National University, Republic of Korea

Cyclopentenone-fused polycyclic compounds are important structural motifs frequently found in natural products and pharmaceutical intermediates. Among various synthetic approaches, the Nazarov cyclization of divinyl ketones represents a powerful strategy for constructing cyclopentenone frameworks, although its application to aryl vinyl ketones remains challenging due to their low reactivity. Herein, we report a trifluoromethylthio (SCF_3)-promoted Nazarov cyclization of α-SCF_3-vinyl (hetero)aryl ketones using trifluoromethanesulfonic acid (TfOH) in dichloromethane (Figure 1). This method enables efficient access to α-SCF_3-substituted cyclopentenone-fused polycyclic compounds in good to excellent yields (up to 96%) under relatively mild conditions. The resulting bromo-substituted products can be readily diversified via Sonogashira and Suzuki cross-coupling reactions, demonstrating their synthetic versatility. Furthermore, density functional theory (DFT) calculations reveal that the α-SCF_3 substituent significantly lowers the activation barrier, thereby promoting the cyclization. This study provides a practical and efficient strategy for accessing a previously unexplored class of SCF_3-substituted polycyclic compounds with potential applications in medicinal chemistry.[1]

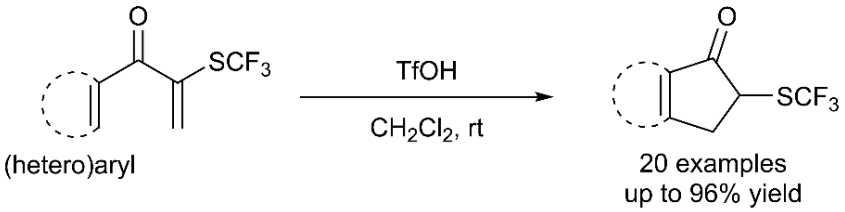


Fig. 1. SCF_3-promoted Nazarov cyclization of α-SCF_3 vinyl (hetero)aryl ketones

[1]Kim, S.; Pyo, Y. J.; Park, G. R.; Kang, H.; Ha, H.-J.; Kim, S. H.; Nam, H. Y.; Cho, D.; Cho, C.-W. *Org. Biomol. Chem.* **2026**, *24*, 360–368.

The 10th EuChemS Chemistry Congress

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Industry Day

ID - O01
From electrons to ensembles: Deep learning that scales DFT, MD, and generative design

Gregor N. C. Simm
Microsoft Research, AI for Science, UK

Microsoft Research AI for Science builds physics-informed AI that turns expensive simulation and limited experiments into fast, reliable decision tools for R&D. We combine first-principles fidelity with learned emulators and generative models to screen and design molecules, materials, and proteins at scale, enabling rapid iteration under practical laboratory and manufacturing constraints. We demonstrate this approach across several R&D bottlenecks: polymer property prediction from quantum data at molecular-dynamics scales,[1] deep-learning exchange–correlation for DFT that reaches chemical accuracy while retaining semi-local efficiency,[2] diffusion-based generation of stable inorganic crystals with tunable property constraints,[3] chemist-aligned retrosynthesis,[4] and rapid emulation of protein equilibrium ensembles that yields free-energy differences consistent with long-timescale MD and experimental stability data.[5] These advances reduce experimental iterations in polymer formulation and processing, accelerate discovery of functional inorganic solids for energy and catalysis, improve route scouting for pharma and fine-chemical manufacturing, and support protein/drug design by exposing cryptic pockets and conformational liabilities.

[1]Simm, G. N. C. et al. SimPoly: Simulation of Polymers with Machine Learning Force Fields Derived from First Principles. arXiv, **2025**. https://doi.org/10.48550/arXiv.2510.13696.
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[3]Zeni, C. et al. A Generative Model for Inorganic Materials Design. *Nature* **2025**, *639* (8055), 624–632.
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ID - O02
Integrated spectroscopy and simulation for absolute configuration assignment

Bernardo de Souza[1], Christoph Riplinger[1]
[1]FACCTs GmbH, DE

Accurately determining the absolute configuration of chiral molecules is essential in pharmaceuticals, catalysis, and materials science. When X-ray diffraction is not feasible, a combination of experimental techniques, such as Nuclear Magnetic Resonance (NMR), Electronic Circular Dichroism (ECD), and Vibrational Circular Dichroism (VCD), combined with sophisticated computational simulations, provides a powerful alternative. Experimental spectroscopy yields essential reference data, while quantum chemical simulations enable predictive modeling of these spectroscopic properties, together allowing the unambigious assignment of the absolute configuration.
Accurate prediction of ECD, VCD, and NMR spectra has historically been challenging. We present a robust computational methodology employing advanced conformational sampling algorithms (GOAT) to generate reliable conformer ensembles[1] as well as computing accurate spectroscopic properties. Our approach specifically targets simulation accuracy comparable to experimental data by systematically addressing three critical best practice areas: (1) extensive and precise conformational searches ensuring comprehensive conformer ensembles; (2) accurate calculation of conformational energies to achieve realistic Boltzmann-weighting;[2] and (3) rigorous prediction of spectroscopic parameters, including key NMR parameters (chemical shifts, J couplings), as well as spectral intensities in ECD and VCD.[3]
Our workflows, carefully validated against outcomes from experiments and from the literature, complement experimental spectroscopy, enhancing the reliability and clarity of stereochemical assignments. Delivered through a user-friendly graphical interface, this integrated experimental-simulation approach has already been successfully adopted in academic and industrial laboratories. By clearly defining and disseminating best practices, our work significantly improves both the accuracy and practical utility of absolute configuration determinations, supporting complex chemical analyses and intellectual property protection. We will present several examples demonstrating how these workflows are currently applied in pharmaceutical companies for real-world structure elucidation challenges.

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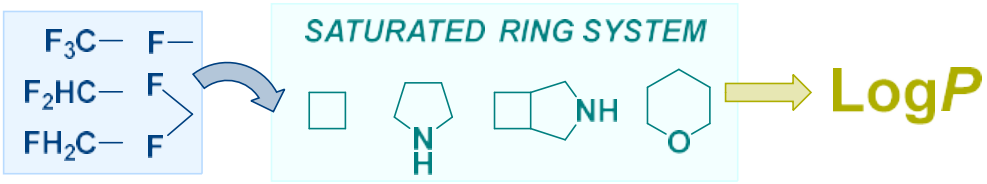
ID - O03

Log*P* *vs* fluorine: Stories from saturated ring systems

Oleksandr Grygorenko[1,2,3], Oleksandr Liashuk[2,3], Kostiantyn Melnykov[1,2], Anton Chernykh[1,4]

[1]Enamine Ltd., UA; [2]Taras Shevchenko National University of Kyiv, UA; [3]Enamine Scientific Research Institute, UA; [4]Institute of Organic Chemistry, National Academy of Sciences of Ukraine, UA

Introducing fluorine into pharmacologically relevant molecules is a widely employed approach in early drug discovery. Among the physicochemical parameters sensitive to fluorination, lipophilicity, commonly quantified by the logarithm of the *n*-octanol/water partition coefficient (Log*P*), is one of the most significant. While the fluorination of aromatic systems is generally associated with an increase in Log*P*, its effect on the aliphatic compounds is considerably less straightforward. This presentation summarizes more than five years of our investigations into the lipophilicity of fluorine-containing saturated carbocyclic and heterocyclic systems, illustrated by a series of representative case studies. In addition, several hypotheses are proposed to explain the experimentally observed trends.



The work was funded by Enamine Ltd and the Ministry of Education and Science of Ukraine.

ID - O04
High-accuracy QM in life sciences: From drug properties to binding modes

Christoph Riplinger[1], Bernardo de Souza[1], Michael Edmund Beck[2,3], Frank Neese[4]
[1]FACCTs GmbH, DE; Bayer AG, DE; [2,3]Technische Universität Dortmund, DE; [4]Max-Planck Institut für Kohlenforschung, DE

Quantum chemical (QM) calculations for life science applications have traditionally been constrained to small model systems, or computationally inexpensive but lower-accuracy methods, due to computational limitations. Most biomolecular modeling approaches rely on empirical parametrization and thus, at least indirectly, on some sort of training, which introduces biases and restricts their applicability. In particular, crucial drug targets such as RNA and metalloproteins often fall outside the scope of conventional methods, requiring extensive parametrization efforts.
Recent advances in quantum chemistry, alongside improvements in computing hardware, have enabled the application of high-accuracy QM methods – such as hybrid density functional theory (DFT) and coupled cluster (CCSD(T)) – to biomolecular systems.[1, 2, 3] These developments now allow for the accurate simulation of ligands in solution as well as in complex biological environments, including their chemical stability, potential degradation pathways, and photochemical reactivity. Moreover, the integration of QM calculations with machine learning models further enhances their predictive power, opening new avenues for drug discovery.
In this talk, we illustrate how state-of-the-art QM approaches are applied across various stages of drug development, from predicting photochemical degradation to elucidating binding mechanisms in metal-containing proteins.

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[2] Beck M.E., Riplinger C., Neese, F., Bistoni G. *J. Comp. Chem*, **2021**, 42, 293.
[3] Kaltschnee L., Pravdivtsev A.N., Gehl M., Huang G., Stoychev G.L., Riplinger C., Keitel M., Neese F., Hövener J.-B., Auer A.A.,Griesinger C., Shima S., Glöggler S. *Nature Catalysis*, **2024**, 7, 1417.

ID - O05
Catalysis at machine speed: Closing the loop from hypothesis to working materials

Ahmed S.M. Ismail[1]
[1]Dunia Innovations GmbH, DE

Catalysts underpin more than 90% of industrial chemical processes and are central to the energy transition, from CO_2 conversion to hydrogen and sustainable fuels. Despite decades of fundamental advances in catalysis science, the translation of new catalyst concepts into industrial deployment remains prohibitively slow, costly, and uncertain. Conventional discovery pipelines rely on sparse datasets, simplified descriptors, and sequential experimentation, resulting in development cycles exceeding 15–20 years and R&D costs in the hundreds of millions of euros.

Here we present a new paradigm for catalyst discovery based on autonomous robotics and AI-driven experimentation that is implemented in Dunia Innovations' Intelligent Research and Innovation System (IRIS). IRIS integrates physics-informed machine learning models, robotic synthesis, device-level electrochemical testing, and closed-loop optimization to enable rapid exploration of high-dimensional catalyst design spaces inaccessible to human-led approaches. In contrast to purely simulation-based methods, IRIS continuously generates high-fidelity experimental data under realistic operating conditions, allowing AI models to learn dynamic structure–reactivity relationships directly from the physical world.

We demonstrate how this approach enables the discovery and optimization of complex multimetallic and alloyed catalytic systems for CO_2 conversion, alkene epoxidation and hydrogen generation, which can also include non-intuitive compositions with emergent activity arising from dynamic surface and alloying effects, consistent with recent advances in operando characterization and theoretical modelling of catalytic state dynamics.[1-3] IRIS can run 50+ autonomous design–make–test–analyze cycles per day. This enables catalyst discovery and scale up to accelerate by more than an order of magnitude while significantly improving reproducibility and scalability.

This work illustrates how autonomous laboratories can transform catalytic science into a data-driven, accelerated industrialized innovation process, which has the potential to accelerate the deployment of catalysts critical to decarbonization and sustainable chemical manufacturing.

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[2]Pessemesse, Q. et al., J. Am. Chem. Soc. (2025), DOI: 10.1021/jacs.5c01968.
[3]Pessemesse, Q. et al., ChemRxiv (2024), "Modelling the Impact of Alloying State Dynamics on-the Reactivity of Group-10-Metal-Gallium Nanoparticles." DOI: 10.26434/chemrxiv-2024-lthtv.

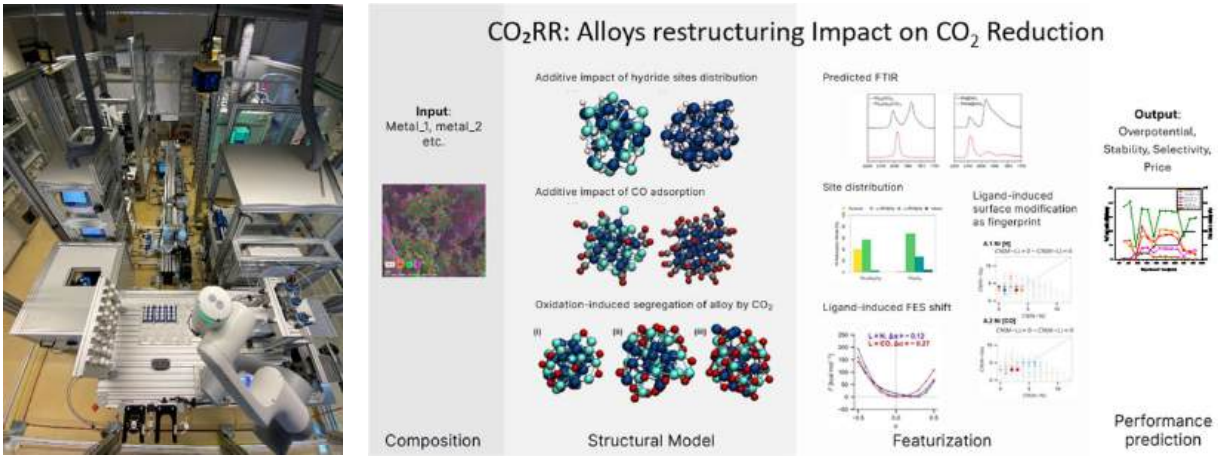

Fig. 1. An image of IRIS Platform (Left). Dynamic modelling approach of catalytic alloy for CO_2 reduction reaction (Right).

ID - O06

Organometallic chemistry in flow: From empirical exploration to rational process design

Oleksandr Andrushko[1,2], Vadim Sham[1,2], Dmytro Lutfullin[1,2], Olexandr Pashenko[3,4], Serhiy Ryabukhin[1,2,3,4], Dmytro Volochnyuk[1,2,3,4]

[1]Enamine Ltd, UA; [2]Institute of Organic Chemistry, NAS of UA; [3]Enamine Scientific Research Institute, UA; [4]Taras Shevchenko National University of Kyiv, UA

Organometallic reagents, particularly organozinc and organolithium species, underpin countless synthetic transformations essential to pharmaceutical and fine chemical manufacturing. Yet their inherent instability, air and moisture sensitivity, and often unpredictable reactivity have long limited the use of these powerful synthetic tools. At the laboratory scale, handling these reagents in batch is straightforward. However, scaling up changes everything. Controlling exotherms across large volumes, maintaining uniform cryogenic conditions, and ensuring reproducibility become increasingly difficult as quantities grow from grams to kilograms.

Continuous-flow technology has emerged as a compelling paradigm for “taming” such chemistry. Precise temperature control, minimal reagent inventory, and confined reaction volumes address many traditional concerns.

Building on our prior work in flow organolithium chemistry, including kilogram-scale directed metalation1 and halogen-lithium exchange processes2, we have systematically expanded into organozinc chemistry with in-house reactor platforms for on-demand reagent generation. Because a successful outcome with a single substrate/reagent/conditions combination tells you little, we have worked toward a comprehensive understanding of the scope and limitations of organometallic reactions in flow by accumulating extensive empirical data.

Our work encompasses both lithium and zinc organometallics across nearly a thousand substrate-reagent combinations, up to multi-hundred-gram scale, providing a foundation for rational process design. We present criteria for substrate selection, guidelines for matching reagent systems to appropriate flow conditions, and indicators that signal likely failure modes. The patterns emerging from systematic screening will allow practitioners to make informed decisions earlier in development and avoid costly dead ends.

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[2]Subota, A., Lutsenko, A., Vashchenko, B., Volochnyuk, D., Levchenko, V., Dmytriv, Y., Rusanov, E., Gorlova, A., Ryabukhin, S., Grygorenko, O. *Eur. J. Org. Chem.* **2019**, *22*, 3636-3648.

ID - O07

The dual mention at the University of Valencia, Faculty of Chemistry: An integrated university–industry formation model

Alicia Monleón-Ventura, Rafael Ballesteros-Garrido, Daniel Tordera, María Teresa Albelda, Maria-Jose Ruiz-Angel, Rafael Ibañez
Faculty of Chemistry, University of Valencia, ES

The Dual Mention Program at the University of Valencia (UVEG) is a regulated educational pathway that integrates university-based academic training with structured, paid professional experience in a collaborating company or institution. This model aims to enhance students' employability by promoting the acquisition of technical and transversal skills aligned with real industrial and professional environments. In accordance with Spanish higher education regulations, the Dual Mention allows a significant proportion of the degree credits to be completed in a work-based learning context, under joint supervision by academic tutors and company mentors. At the UV, this pathway has been implemented in selected degree programmes, such as the Degree in Chemistry, in collaboration with leading organizations in the sector, fostering a closer link between university education, innovation, and the labour market. Herein, we present and analyse the results obtained after two years of implementation of the Dual Mention program.

ID - SKN1

Sustainability as a business driver

Tal Shapira[1,2]

[1]Triple W, BE; [2]Triple W, USA

At TripleW, we often get asked how we view the massive global challenge of food waste. To explain our vision we like to look back at the 19th-century Petroleum Revolution.

Before the 1850s, "rock oil" was considered a valueless nuisance - a messy byproduct that ruined farmland and contaminated wells. It only became the foundation of the modern world when refiners figured out how to "crack" that valueless sludge into high-value energy and materials.

Today, food waste is our "rock oil."

Most see it as a costly liability to be buried or burned. At TripleW, we see it as an abundant, untapped "ore." We aren't just managing waste; we are the refiners of the 21st century. By converting this carbon-rich food waste into lactic acid, we are creating the foundational building blocks for the next generation of sustainable PLA bioplastics.

ID - SKN2

Bernd Haveresch - Ammobia

Global ammonia demand is projected to quadruple until 2050, driven by fertilizers and, in particular, by clean maritime fuel and energy storage. Yet conventional Haber-Bosch production remains carbon-intensive, capital-heavy, and vulnerable to supply chain disruptions.

Ammobia has developed a novel low-pressure ammonia synthesis technology achieving record-high single-pass conversion at at a fraction of the typical operating pressure.

Independently validated the technology comes with a 2× capex reduction potential.

Ammobia's modular, feedstock-agnostic design enables decentralized production close to renewable energy sources or demand centers. The company is now advancing from TRL 6 toward an industrial demonstration and a first commercial plant by 2028–2029, actively seeking partners and project locations in Europe and beyond.

ID - SKN3
Reactor design according the KISS principle: Keep It Simple and Scalable

Koen Van Aken
Creaflow, BE

Due to its proven advantages, flow chemistry is continuing to cement its position in academia and industry. However, despite over a decade of R&D efforts, some challenges remain in the areas of handling multiphase processes, alternative energy input and scale-up.

Therefore, a platform reactor technology (*i.e.,* COSTA™ Technology) has been developed featuring the arrangement of static mixing elements in a linear process channel combined with an oscillatory flow regime (Figure 1). The synergetic combination of reactor geometry and pulsatile flow results in a plug flow behavior with intense mixing regardless of the net flow rate and excellent thermoregulation.

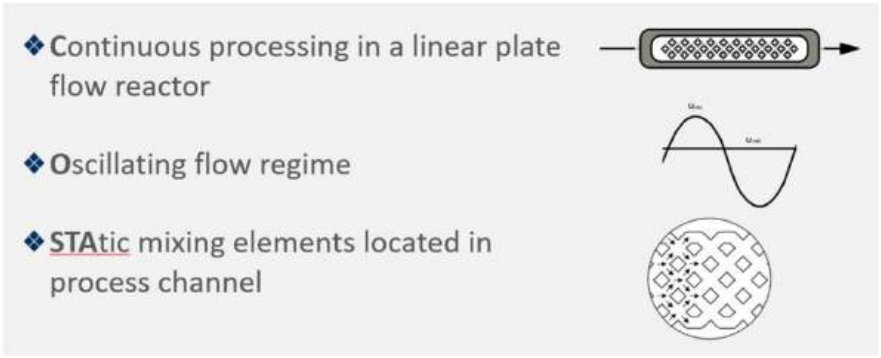

Fig. 1. Working Principle of the COSTA™ Technology

Several reactor types has been engineered based on this platform technology. These systems enable linear scale up as critical process characteristics, such as mass- and energy-transfer, residence time distribution and pressure drop, are not affected. To demonstrate the scope of this technology, a series of (multi-phase) photo- and electrochemical applications will be presented highlighting the unique capabilities of this innovative reactor design.

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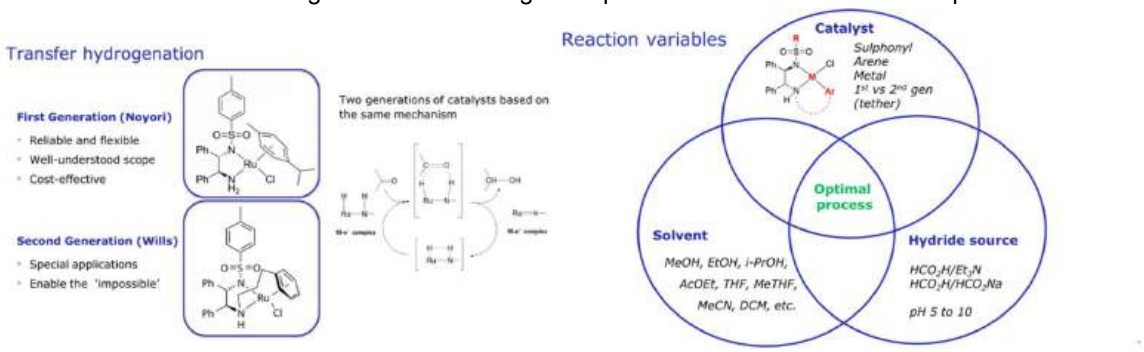
ID - O08

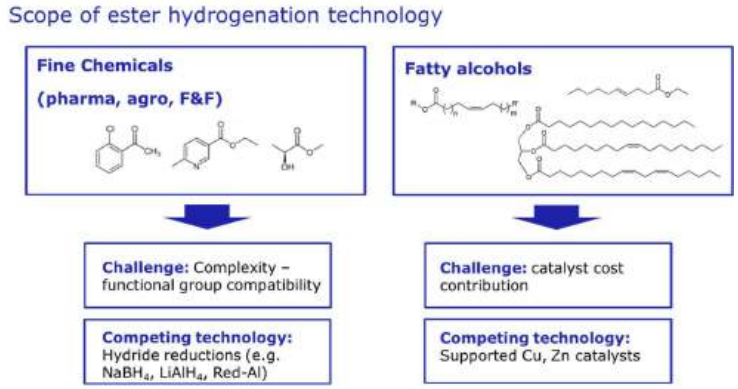
Asymmetric transfer hydrogenation and homogeneous ester hydrogenation at Johnson Matthey

Stephen Roseblade[1], Damian Grainger, Antonio Zanotti
[1]Johnson Matthey plc, Cambridge Science Park, UK

Asymmetric transfer hydrogenation using first- and second-generation catalysts available at JM will be discussed.[1] Second generation catalysts offer advantages, allowing lower loadings and easier product purification. Second generation catalysts also provide more robust processes and improved functional group tolerance, helping to facilitate their application in complex molecules synthesis.[2] The factors to be taken into account and assessed during reaction screening and optimisation case studies will be presented.



Homogeneous ester hydrogenation has been investigated extensively in academic and industrial research groups. JM have an exclusive license to Gusev Ru catalysts for the reduction of esters to alcohols. The key characteristics and scope of this technology will be outlined.[3]



Recent research results using ruthenium carboxylate catalysts and their application to the productive hydrogenation of fatty esters will be presented.[4] Material on the **carbon footprint** of a basic transfer hydrogenation catalyst, and the sustainability of platinum group metals in the fine chemical industry, will also be presented.[5]

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ID - O09

Unlocking point source CO_2 capture from low concentration flue gas – A hybrid technology

Fanni Sypaseuth[1], Aurélien Vantomme[1], Samuel Thiry[1]
[1]ARK Capture Solutions, BE

The role of carbon capture in decarbonizing power generation and industry is well documented in the literature. In power generation, carbon capture can help decarbonize existing thermal assets and provide firm, low-carbon electricity where renewables alone may not guarantee system reliability.[1] In the chemical industry, carbon capture is essential to abate process emissions from fossil-based feedstocks and reaction chemistry that cannot be fully eliminated through electrification or efficiency measures.[2] Many of these emissions come from dilute flue-gas streams, such as gas-fired power plants and combustion processes in steel, cement, and glass. Capturing CO_2 from these low-concentration streams is more energy-intensive and costly than from high-purity process streams with today's technologies. This makes them among the hardest sources to abate cost-effectively.[3]

Today, there is no widely deployed commercial option that captures CO_2 from dilute flue gas at low cost and low energy use without relying on large solvent-based absorption units. Many customers are reluctant to adopt amine systems because they are capital-intensive and complex to operate, require significant steam and cooling utilities, and introduce issues such as solvent management, degradation, corrosion, and emissions control.

Herein, we present a novel solvent-free hybrid carbon capture technology that can recover CO_2 from low-concentration flue-gas streams (4 – 15%) at significantly reduced energy demand and capture cost. The captured CO_2 is delivered as a high-purity product (> 99%) that meets established specifications for transport, geological storage and utilization.

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ID - O10

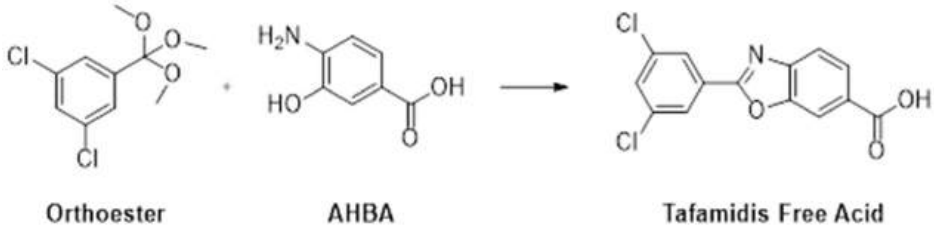
Development of a One-Step Continuous Manufacturing Process for Tafamidis API via Enabling-Chemistry & FAST Technology

Ramulu Akula[1], Declan Cusack[1], Joseph Keane[1], Piotr Mytych[1], Chris Nottingham[1], Jonathan White[1], Patrick Sweeney[1]

[1]Small Molecule Technology, Global Technology Engineering & Launch, Pfizer Global Supply (SMT-GTEL, PGS), IE

A novel one-step continuous manufacturing process has been developed and optimized for the active pharmaceutical ingredient (API) of Tafamidis. This *Flexible API Supply Technology (FAST)* approach builds upon one-step batch chemistry that was previously developed in the Pfizer Process Development Center [1] and enables **reactive crystallisation in flow**, directly coupling 4-amino-3-hydroxybenzoic acid (an established starting material) with a newly developed orthoester intermediate in the presence of catalytic trifluoroacetic acid (TFA) and ascorbic acid. The entire API forms in a single step within a cascade of continuous stirred-tank reactors (CSTRs). Proof-of-concept trials confirmed an isolated Tafamidis yield of ~85%, with product quality equivalent to the traditional multi-step batch syntheses [2]. Extended 24-hour runs demonstrated steady operation with minimal intervention, leveraging advanced process analytical technology and real-time monitoring to maintain a state of control. **Key process metrics show transformative improvements over batch processing:** the 1-step continuous method will reduce overall production time from ~107 days to ~31 days for a typical campaign and eliminates two isolation points, markedly **reducing solvent waste** (by >95%) and **shrinking equipment footprint** (total reactor volume ~4,430 L vs 176,480 L). The process was successfully scaled in the Kilo Technology Lab using a 3×1 L CSTR train, producing 1 kg of API per day. Comprehensive safety evaluations indicated no significant exotherms or off-gassing, supporting the inherent safety of this intensified process. In summary, the second-generation Tafamidis FAST process delivers **significantly shorter cycle time, higher sustainability, and robust performance** relative to the batch route. This work demonstrates the potential of Pfizer's FAST continuous technology when applied to marketed APIs, and contributes to future development and commercialisation of flow processes in pharmaceutical manufacturing [3, 4].

Fig. 1. Schematic of the acid-catalysed one-step chemistry to make Tafamidis free acid API; Visual of the balancing of AHBA conversion across the CSTRs to limit the supersaturation via temperature change or TFA addition to prevent sub-surface fouling



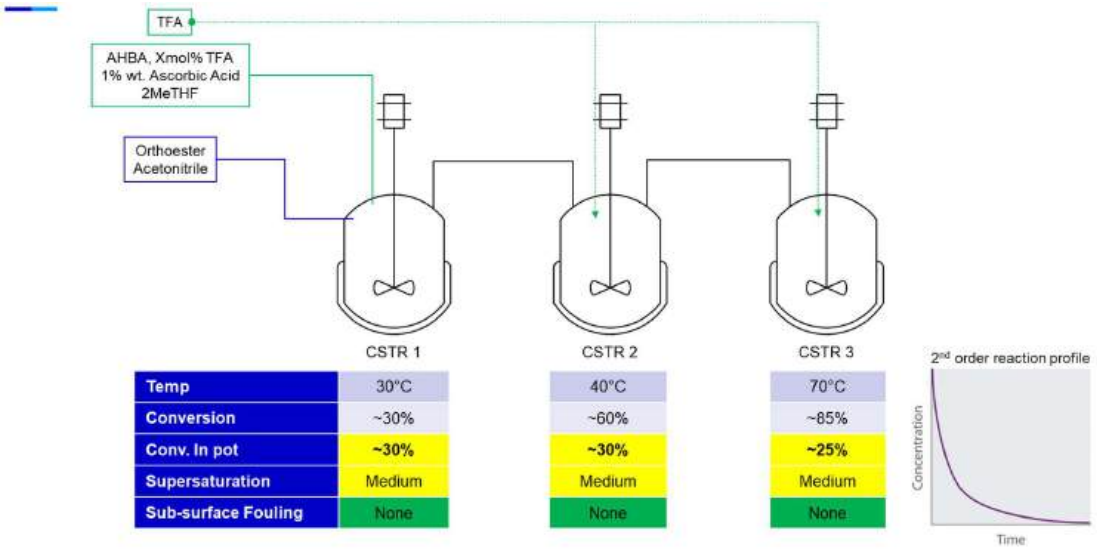


Table 1 – Comparison of current batch process vs. new 1-step continuous FAST process for Tafamidis API (for a 625 kg production campaign)

Parameter	Batch Process	Continuous FAST Process
Synthesis steps	3 steps (multi-stage)	1 step (end-to-end)
Total reactor volume required	~176,480 L	~4,430 L
Production time for 625 kg API	~107 days	~31 days
Solvent waste generated	~435,000 kg	~15,000 kg
Isolated intermediate streams	2 (solid isolations)	0 (none)
Isolated yield (API)	~85%	~85%
Product quality/purity	Equivalent to current	Equivalent (no change)

The authors gratefully acknowledge the contributions of SMT-GTEL colleagues (Process Development Center & Kilo Technology Lab teams), Manufacturing Intelligence & Technology Transformation (MITT-GTEL) and Chemical R&D (Groton FAST team) for their expertise and support. We also thank the Manufacturing Technology Development Centre (Singapore) for kinetic modelling and the Pfizer Global Operations teams for facilitating scale-up trials. *(This project was internally funded by Pfizer; no external funding was received.)*

[1]Curran, S & O'Neill, P. (2021). Efficient process for making 6-carboxy benzoxazole derivatives (WO 2021/124158 A1) PCT/IB2020/062040.https://patentimages.storage.googleapis.com/b1/62/bc/fd792408deb628/AU2020406455A1.pdf
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ID - SKN4
From waste to strategic resource: Scaling circular chemistry in Antwerp and Europe

Karl Huts, CEO
Indaver Group

Waste is dirty? No, it's just waiting for the right chemistry. The transition towards a circular chemical industry requires moving beyond conventional value chains and addressing complex, heterogeneous waste streams that still contain significant material and energy value. Retaining this value within the system is essential to reduce dependency on virgin resources and to strengthen Europe's industrial resilience.

At Indaver, this challenge is at the most fundamental level: the molecule. By understanding waste streams at their chemical building blocks, it becomes possible to recover maximum value, transforming them into secondary raw materials, energy and high-value products such as precious metals. This integrated approach facilitates full valorisation, rather than partial treatment.

With its industrial footprint in Antwerp and across Europe, Indaver demonstrates that this model is operational at large scale. Flagship sites and installations combine advanced thermal treatment, chemical processing and resource recovery technologies to convert complex waste streams into multiple valuable outputs. Beyond material recovery, this includes the generation and distribution of energy through heat and steam networks, as well as the integration of renewable energy assets such as solar parks within the port ecosystem.

Continuous investment in innovation further accelerates this transition. The new Plastics-to-Chemicals installation in Antwerp exemplifies how end-of-life plastics can be converted into chemical feedstock, reinforcing the role of Antwerp as a frontrunner in circular chemistry and as a blueprint for Europe.

However, technological capability alone is not sufficient. Industrial regions such as Antwerp are increasingly confronted with regulatory complexity, including evolving frameworks around PFAS and other Substances of Very High Concern, and the absence of a consistent level playing field within Europe. Diverging frameworks and policy uncertainty risk slowing down the deployment of circular solutions. Aligning innovation with a coherent regulatory framework is critical to fully realise Europe's circular ambition.

ID - SKN5
Closing the loop for precious metals from complex industrial waste streams

Florence Luyten
Indaver

Precious metals such as palladium (Pd), ruthenium (Ru), iridium (Ir), platinum (Pt), and rhodium (Rh) are critical elements for the agrochemical and life sciences industries, underpinning catalysis for production of pharmaceuticals, electronics and advanced materials. At the same time, their primary extraction is highly energy-intensive, geopolitically sensitive and environmentally burdensome. Recovering these metals from industrial liquid waste streams therefore represents both a strategic necessity and a circular opportunity.

While the industry is familiar with recovery from solid matrices such as spent catalysts, a less widely recognised reality is that today's technologies also enable efficient recovery from complex liquid waste streams, such as mother liquors and aqueous phases from pharmaceutical and fine / agro-chemical, electronics production. This creates significant potential, as valuable metals are still frequently lost in liquid production flows.

Indaver has developed an integrated approach to recover precious metals from liquid waste streams on a large industrial scale. A dedicated recycling installation in Antwerp (Belgium) handles streams typically characterised by both high and low concentrations and complex compositions. By combining advanced thermal and physico-chemical processes, valuable precious metal are concentrated and converted into recoverable forms, while hazardous components are safely removed.

Downstream refining enables the recovery of high-purity metals suitable for reintroduction into industrial value chains. Compared to primary mining and refining, Indaver's recovery routes reduce CO_2 emissions by up to 95%, depending on the metal and process conditions, while also significantly lowering energy use and reducing reliance on virgin raw materials.

Indaver is pioneering in the field of precious metals recovery from liquids. With 10 years of experience and selectively combining the most cost-efficient operational techniques, Indaver offers a tangible pathway towards circularity and resource resilience.

ID - SKN6
From lab to industry: Innovating for sustainable chemistry

Eric de Deckere, Innovation Executive Director
Cefic (European Chemical Industry Council)

It is no secret that the chemical industry is already transforming and must continue to do so rapidly to meet climate and sustainability goals. Meeting this challenge continuously creates new opportunities for researchers to turn science into real-world impact. This Cefic session offers students and early-career scientists a snapshot of how innovation can move from lab to industry.

Key topics:

- Improving sustainability and safety performance of processes and products:
    - Scaling up non-fossil feedstocks (bio-based, waste-derived, carbon capture and utilisation – CCU);
    - Optimising circular solutions, including chemical recycling.

- Applying Safe and Sustainable-by-Design (SSbD) as an innovation framework for the chemical value chain;
- Advancing impact assessment through Cefic's Long-Range Research Initiative (LRI) funding programme, bridging science and industry.

What you will gain:

- Insight into industry research careers;
- Understanding of skills in demand;
- Examples of real-world application of research.

About Cefic and Cefic-LRI

Cefic is the forum of large, medium and small chemical companies across Europe, which provide 1.2 million jobs and account for approximately about 13% of world chemicals production.
Cefic-LRI is Cefic's Long-Range Research Initiative Programme which funds research to address societal challenges with science to improve safety and sustainability of chemicals.
LRI has awarded approximately €90 million to over 250 projects that address European public health strategy priorities.

ID - SKN7

Great British Chemicals: Towards a resilient chemicals industry

Helen Pain - Great Britisch Chemicals

Great British Chemicals is a National Research & Innovation Centre for Sustainable Industrial Futures. Funded by EPSRC & NERC the centre will unite the UK chemical industry, academic researchers and policy makers to advance innovative, scalable and sustainable technology solutions for defossilising chemicals manufacturing. We aim to create people-focussed opportunities to truly shape sustainable carbon management.

ID - SKN8
Plasma based CO_2-CO conversion

Marjon Willekens
D-CRBN, BE

D-CRBN has a proprietary modular and scalable plasma technology capable of splitting the CO_2 molecule into CO or CO_2 + CH_4 (e.g. biogas) into (bio)syngas, all in a fully electrified gaseous phase, without solvents or catalysts. The CO or syngas is then turned into added-value chemicals, such as e-fuels, organic acids, polymers, etc., and used as feedstocks for the chemical, petrochemical, maritime, and metallurgical industries, among others. Our aim at D-CRBN is not only to decarbonize industries by eliminating their point source emissions but also to replace fossil feedstocks with CO_2 recycled added value chemicals. This technology can provide strategic and decentralized resource independence to territories and industries that currently depend on oil and natural gas derivatives for their processes.

The 10th EuChemS Chemistry Congress

12 - 16 July 2026

Antwerp, Belgium

Symposia, Mini-Symposia & Workshops

S - D1 - 1
Strengthening Europe-Taiwan collaboration in chemical sciences

Scientific collaboration between Europe and Taiwan in chemical sciences has grown steadily over the past decade through complementary expertise, shared scientific interests, and strong institutional support. Building upon these successful interactions, this symposium aims to further strengthen connections between the European and Taiwanese chemical communities and to explore new opportunities for long-term collaboration.

The symposium will introduce Taiwan's chemical research ecosystem, including international collaboration mechanisms supported by the National Science and Technology Council (NSTC), major research institutions, and the activities of the Chemical Society of Taiwan in promoting global engagement. Participants will gain insights into existing Europe-Taiwan research partnerships, funding opportunities, and experiences from internationally active researchers.

The Taiwanese delegation represents a broad spectrum of chemical sciences, spanning molecular materials, supramolecular chemistry, organometallic chemistry and catalysis, energy and sustainability, chemical biology, medicinal chemistry, and structural biology. Through a series of research highlights and discussions, the symposium seeks to identify complementary strengths, foster new scientific interactions, and establish sustainable frameworks for future collaboration.

By bringing together researchers from Taiwan and Europe, this symposium provides a platform for scientific exchange, partnership building, and the development of enduring collaborations that will advance chemical sciences and address global challenges in the years ahead.

Agenda

Time	**Program / Speaker**
Phase I. Building Connections and Collaboration Frameworks	
14:00-14:10	Opening Remarks | Vera Meynen
14:10-14:20	Overview of the Chemical Community in Taiwan | Jye-Shane Yang
14:20-14:35	Taiwan–Europe Bilateral Cooperation Mechanisms and Research Platforms | Chun-Cheng Lin
14:35-14:50	Experiences and Perspectives on Europe–Taiwan Research Collaboration | Ching-Wen Chiu
14:50-15:00	Research and Academic Life in Taiwan: An International Researcher's Perspective | Manuel Maestre-Reyna
Phase II. Research Highlights and Collaboration Opportunities	
15:00-16:00	Short Oral Presentations by Taiwan Delegates

Mechanochemistry for sustainable synthesis: From hard materials to soft matter

The mini-symposium is expression of the EuChemS Professional Network (PN) on Mechanochemistry, created in 2023. The symposium seeks to raise awareness of mechanochemistry as a versatile strategy for Safe and Sustainable by Design (SSbD) synthesis, complementing the subject matters transversally covered across the eight ECC-10 congress themes.
It will highlight the multidisciplinary character of mechanochemistry and its largely untapped potential for innovation in sustainable synthesis and its potential of application in different areas of chemical sciences. Invited speakers were defined upon consultations with the members of the EuChemS PN on Mechanochemistry, considering criteria of inclusion, diversity, gender balance, geographic and scientific background distribution. Subject matters of the symposium will cover material synthesis, organic mechanochemistry, crystal engineering, life cycle assessment (LCA) and techno-economic analyses (TEA) approaches for mechanochemistry, transversally complementing the eight ECC-10 main congress themes.
Overall, the mini-symposium aims to promote sustainable scientific and technological solutions by fostering interdisciplinary collaboration and knowledge exchange, supporting the development of mechanochemistry, and encouraging interaction between early-career researchers, newcomers to the field, and established experts within a growing international community.

S - D2 - 1A

Enhancing asymmetric organocatalysis and metal catalysis through mechanochemistry

Radovan Šebesta

Comenius University Bratislava, Faculty of Natural Sciences, Dept. of Organic Chemistry, Mlynská dolina, Ilkovičova, Bratislava, Slovakia

Combining asymmetric organocatalysis with mechanochemistry offers a powerful route to more sustainable and efficient synthesis. In our recent study, a mechanochemical, organocatalytic domino Mannich reaction incorporating fluorination delivered oxindolyl fluoropyrazolones in high yields, excellent enantioselectivities, and markedly reduced reaction times.[1] Likewise, formal organocatalytic cycloadditions performed under ball-milling conditions provided diverse chiral pyranes,[2] and tetrahydroquinolines with high efficiency.[3] We also report the first mechanochemical atroposelective transformation, enabling access to axially chiral biaryls.[4] Across these processes, liquid-assisted grinding proved critical, with the choice of additive exerting a strong influence on both yield and enantioselectivity.

Metal-catalyzed cross-coupling reactions are indispensable for constructing complex molecular architectures, yet their reliance on sensitive transition-metal catalysts and organometallic reagents remains a key limitation. Mechanochemistry offers a compelling strategy to overcome these challenges.

In this context, we investigated the mechanochemical cross-coupling of organozinc pivalates with aryl halides.[5] Building on this approach, we generated additional organozinc intermediates in situ— Reformatsky enolates— under mechanochemical conditions, followed by Pd-catalyzed cross-coupling in the same environment.[6] More recently, we explored arylthianthrenium salts as alternative electrophiles in Pd-catalyzed cross-couplings with organoboron and organozinc reagents.[7,8] We also demonstrated that Pd-catalyzed carbonylation of aryl halides with amines and phenols can be achieved mechanochemically. A key enabling factor in these transformations is the use of solid $FeBr_2(CO)_4$ as a convenient CO source.[9] Overall, our results highlight that mechanochemistry enables more sustainable cross-coupling processes, allowing reactions to proceed under ambient conditions and in air—even with otherwise sensitive organometallic reagents.

This work was supported by the Slovak Grant Agency VEGA, grant no. VEGA 1/0445/24 and the Slovak Research and Development Agency under the contract APVV-22-0167.

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[2]Peňaška, T., Modrocká, V., Stankovianska, K., Mečiarová, M., Rakovský, E., Šebesta, R. *ChemSusChem*, **2022**, *15*, e202200028.
[3]Kisszékelyi, P., Doblejová, T., Rakovský, E., Šebesta, R. *Chem. Eur. J*. **2025**, *31*, e02466.
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S - D2 - 1B

Local structural disorder–magnetism relationships in nanostructured complex oxides prepared by mechanochemical synthesis

V. Šepelák
Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

The interplay of magnetism and structural disorder in nanostructured complex oxides is a fascinating subject of recent interest.[1] The present work reviews a one-step mechanochemical synthesis and magnetic properties of magnetoceramics with a variety of structure types (cubic spinel, orthorhombic olivine, perovskite, hexagonal structure, double perovskite). The case studies are presented, focusing on recent progress in a fundamental understanding of the structural disorder–magnetism relationships in “interface-controlled” complex oxides prepared by mechanochemical routes. The far-from-equilibrium structural disorder in iron containing magnetic nanomaterials is studied by means of ^{57}Fe Mössbauer nuclear probe spectroscopy. The functional behaviour of mechanochemically synthesized oxides is characterized by SQUID measurements. Selected examples of the separation of interfacial/surface effects from bulk effects in oxide nanoparticles are presented. It is demonstrated that interfacial effects in the mechanochemically synthesized ceramics may result either in an enhancement of magnetic behaviour or in its degradation, *i.e.*, in a desired or undesired magnetic property modification, when compared to magnetism of their bulk counterparts prepared by a conventional ceramic method.

Acknowledgements: The present work is supported by the DFG (project SE 1407/4-2).

[1]García, F.; Senna, M.; Šepelák, V. *RSC Mechanochem.* **2025**, 2, 499 – 502. DOI: 10.1039/D5MR90017D

S - D2 - 1C

Life cycle assessment of active pharmaceutical ingredients by mechanochemistry: Case studies in ball milling, RAM and TSE

Sabrina Spatari[1], Yaron Aviezer[1], Michael Patrascu[1], Christos Chatzagiannis[2], Evelina Colacino[2]
[1]*Technion – Israel Institute of Technology, Israel;* [2]*Univ. Montpellier, France*

Mechanochemical processes hold great potential for reducing environmental impacts within the pharmaceutical industry by eliminating solvents when manufacturing active pharmaceutical ingredients (API). Here, we demonstrate the use of environmental life cycle assessment (LCA) and techno-economic analysis (TEA) to evaluate the benefits and tradeoffs of using mechanochemical preparation of World Health Organization (WHO) essential medicines by ball milling, twin-screw extrusion (TSE) and resonant acoustic mixing (RAM) and we benchmark production relative to traditional production of APIs by solvent-batch processes. Our findings illustrate benefits in life cycle environmental, economic and productivity metrics for several processing regimes, where depending upon the API, specific mechanochemical processes were found to achieve preferred performance over multiple impact assessment categories. While mechanochemical processes are still evolving, this early-stage evaluation posits that with further process optimization and industrial learning, mechanochemical processes are likely to be economically competitive while reducing environmental waste.

The authors gratefully acknowledge IMPACTIVE (Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients), the research project funded from the European Union's Horizon Europe research and innovation programme (European Health and Digital Executive Agency) under grant agreement No. 101057286.

S - D2 - 1D

Mechanochemistry-driven crystal engineering and supramolecular chemistry of antibiotics and anti-cancer drugs

Vânia André[1,2]

[1]CQE-IMS, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal; [2]Associação do Instituto Superior Técnico para a investigação e o desenvolvimento (IST-ID), Lisbon, Portugal

Crystal engineering and supramolecular chemistry offer powerful ways to enhance the performance of currently available drugs, improving solubility, bioavailability, stability, and ultimately therapeutic efficacy. Bearing in mind that antimicrobial resistance (AMR) is accelerating faster than the ability to develop new drugs, creating an urgent need for strategies that can revitalize existing antimicrobials by unveiling more efficient drug forms[1-4], major emphasis of our work has been put into antimicrobials. Polymorphs, pharmaceutical cocrystals, antibiotic coordination frameworks, and bio-inspired metal–organic architectures have demonstrated the ability to boost antimicrobial activity or unlock new modes of action. Nevertheless, also anticancer drugs can benefit from these approaches for the development of new drug forms with enhanced properties and/or activity.
Mechanochemistry sits at the center of these advances. It provides a clean, solvent-minimal, and highly versatile platform for synthesizing all these solid forms, from polymorphs to cocrystals to metal–organic assemblies. Its efficiency, scalability, and alignment with green-chemistry principles make mechanochemistry not just a method of election, but a transformative tool for antibiotic solid-form discovery.
This presentation highlights mechanochemical results obtained with a diverse set of antimicrobial agents, including praziquantel, tazobactam, nalidixic acid, and silver–sulfadiazine, alongside newly designed molecules. Recent work on anticancer drugs, in particular lenalidomide,[5] is also going to be presented, where mechanochemical crystal engineering has opened new pathways for possible tuning therapeutic performance. Together, these examples illustrate how mechanochemistry can reshape the solid-form landscape of both antimicrobial and anticancer compounds, offering a powerful platform to address some of today's most pressing therapeutic challenges.

Acknowledgements: The author acknowledges IMPACTIVE (Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients), the research project funded from the European Union's Horizon Europe research and innovation programme (European Health and Digital Executive Agency) under grant agreement No. 101057286. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or (European Health and Digital Executive Agency). Neither the European Union nor the granting authority can be held responsible for them. Fundação para a Ciência a Tecnologia and Plano de Recuperação e Resiliência (PRR) are acknowledged for funding projects UID/00100/2025 (DOI 10.54499/UID/00100/2025); UID/PRR/00100/2025 (DOI 10.54499/UID/PRR/00100/2025); UID/PRR2/00100/2025 (DOI 10.54499/UID/PRR2/00100/2025), and LA/P/0056/2020 (DOI 10.54499/LA/P/0056/2020), and the contract 2023.15700.TENURE.042 under the Scientific Employment Stimulus- FCT-Tenure and Plano de Recuperação e Resiliência (PRR) n.º 02/C06i06/2024 funding.

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S - D3 - 1
Porous materials at the frontier of sustainable catalysis

Porous materials act as highly efficient catalysts by providing immense internal surface areas, high selectivity, and structural stability. As global industries seek cleaner processes and more efficient resource use, these materials stand at a pivotal intersection of fundamental science and practical impact.
This symposium, hosted by *ACS Central Science*, will feature talks from outstanding researchers at various career stages and will highlight the catalytic concepts facilitated by porous materials from both experimental and theoretical perspectives and how they address challenges that remain in scaling, integration, and long-term sustainability

S - D3 - 1A
Electronic transport and single-site catalysis in Covalent organic frameworks

Thomas Bein
Dept. of Chemistry and Center for NanoScience, University of Munich (LMU), Munich, Germany

Covalent organic frameworks (COFs) are crystalline, porous, and conjugated materials that are attractive for sustainable energy because their ordered pores can support efficient charge transport and catalytic functions. We will discuss both transport phenomena and single-site catalytic activity in COFs. First, we establish that a 2D COF thin film can support very fast excited-state transport – remote-detected time-resolved photoluminescence and optical pump–terahertz probe measurements reveal early free-carrier diffusion followed by bound-state formation, identified as excitons, with lateral diffusion coefficients as high as 4 $cm^2 s^{-1}$ and diffusion lengths reaching several hundred nanometers, even across grain boundaries.[1]
Second, a dibenzochrysene-based COF was established as a rigid, crystalline host for atomically positioned Re(I) centers, creating a hybrid photocatalyst for CO_2 reduction with high CO evolution rates and strong photostability.[2] Third, a phenanthroline-based 2D COF electrocatalyst bearing Mn(I) single sites was integrated into a catholyte-free membrane-electrode-assembly cell, where it achieved a high turnover frequency while suppressing Mn–Mn dimerization and maintaining stable high-potential operation.[3] Finally, we will discuss strategies for tailoring optoelectronic processes in COFs towards desired applications, including stacking effects,[4] chromophore design,[5] donor-acceptor architectures,[6] and structurally dynamic lattices.[7]

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S - D3 - 1B
New vistas on zeolite catalysis for organic reactions

Dirk De Vos
cMACS, Dept. of Microbial and Molecular Systems, KULeuven Leuven, Belgium

While zeolites are foremost known for their role in adsorption and petrochemical catalysis, their porous architecture and functionality enable a wide range of topical reactions that are useful either for the synthesis of specialty chemicals, or in the quest for carbon circularity. A first series of examples focuses on active metal sites in zeolites. Ionic **Pd sites** inside zeolite Beta catalyze the selective oxidative biaryl coupling of substituted aromatics like toluene or anisole. Remarkably, the zeolite framework strongly directs the C-H activation process towards a *para-para* selective coupling, favouring 4,4'-coupled isomers like 4,4'-bitolyl.[1] **Ti sites** on the periphery of delaminated zeolites are capable of selectively introducing ketone functions into polyethylene.[2] These oxidative, C-H activating reactions proceed without inducing scission in the polymer backbone. We will show that the ketonized polyethylene can serve as a precursor for polyesters and polyamides, with the ester and amide groups incorporated in the chain. This makes the polyethylene infinitely recyclable. In a last example, reducing **metallic functions** can be entrapped inside zeolite hosts, and in this way, uniquely selective catalysts for alcohol amination can be designed, for instance for the selective amination of propanol to mono- and dipropylamine, fully suppressing the formation of less desired tertiary amines.
In a second group of zeolite applications, the zeolite is used as a matrix to **compartmentalize the reaction space**. In shuttle reactions like transfer hydrocyanations, a Pd-loaded zeolite can be used in combination with a homogeneous Pd HCN-transfer catalyst to drive the equilibrium of this isodesmic reaction to the desired side.[3] For instance, when the homogeneous catalyst uses propionitrile as a HCN-donor for the hydrocyanation of a complex olefin, a zeolite pulls the equilibrium by converting the ethylene co-product of the transfer reaction. With an analogous equilibrium-driving concept, a combination of a zeolite and a homogeneous carbonylation catalyst can perform hydroformylations with CO_2 in remarkably mild conditions.[4]

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S - D3 - 1C

Hybrid QM/QM studies of the electronic structure, d-d excitations, and spin crossover in metal-organic frameworks containing transition metal ions

Elena Besley
School of Chemistry, University of Nottingham, UK

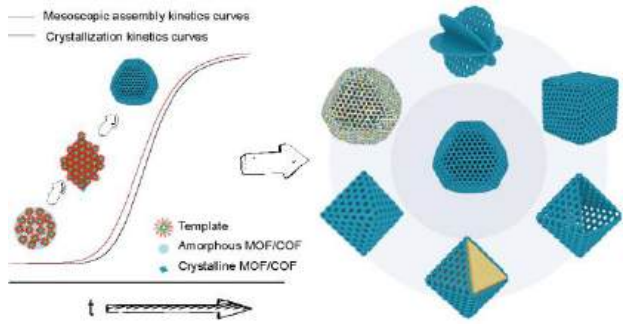
The electronic structure of metal−organic frameworks (MOFs) containing transition metal (TM) ions represents a significant and largely unresolved computational challenge due to limited solutions to quantitative description of low-energy excitations in open d-shells. These excitations underpin the magnetic, catalytic, and sensing properties of TM MOFs, including the observed remarkable spin crossover phenomenon. We introduce a hybrid QM/QM method, called the periodic effective Hamiltonian of crystal field (pEHCF) method [Molecular Physics 2022, 121, e2106905], which is based on the separation of crystal structure into d- and s,p-subsystems treated at different levels of theory. We test the performance of pEHCF on a series of M-MOF-74 (M = Fe, Co, Ni) structures and compare the computational predictions to experimental data on magnetic properties and Mössbauer spectra [J. Phys. Chem. C 2023, 127, 21749]. We also show how pEHCF performs in challenging calculations of the electronic structure of high-spin and low-spin electron configurations of MOFs which exhibit unusual spin crossover behaviour [J. Chem. Phys. 2025, 163, 054117].

S - D3 - 1D
Controllable synthesis of mesoporous crystalline frameworks

Dongyuan Zhao[1]
[1]Laboratory of Advanced Materials, Fudan University, Shanghai, China; [2]College of Energy Materials and Chemistry, Inner Mongolia University, China

Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) have emerged as classical crystalline porous materials, showing a great promise in various areas such as catalysis, gas storage and separation. Owing to the inherent microporosity, the applications of such frameworks involving large molecules are greatly hindered. The synthesis of mesoporous MOFs/COFs is hampered by imbalance in structural tension at the micro-scale of the crystalline MOF framework and the meso-scales of surfactant-composite self-assembly. Here, we have demonstrated a cooperative assembly strategy by regulating crystallization kinetics and template interactions, enabling the formation of crystalline mesoporous MOFs/COFs with tunable architectures. This approch has been extended to more complex hierarchical porous networks. A library of meso-MOFs with a wide range of morphologies (cubes and 2D nanosheets), compositions and architectures (hollow and core-shell structures), have been constructed. By integrating mesoscale channel networks while preserving long-range order and site-definability at the micro-scale, we have successfully reduced diffusion resistance and enhanced interfacial exchange, thereby promoting efficient combination of reaction kinetics and ion transport with internal active centers. The ordered mesoporous MOFs/COFs offer unique advantages in cross-scale mass transport and improved site availability, providing structurally robust, high-flux platforms for membrane-based separations, selective transport.
Fig. 1 Scheme illustration of the formation of the mesoporous MOFs/COFs.

Key Words: Mesoporous Materials; Metal-organic frameworks (MOFs); covalent organic frameworks (COFs); self-assembly



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S - D3 - 1E
Assembly of Hybrid nanoporous materials for advanced functionalities

Mónica Giménez Marqués, Jesús Cases Díaz, Jana Glatz, Thibaut Le Huec
Insituto de Ciencia Molecular, Universitat de València, Paterna, Spain

Hybrid nanostructures composed of multiple chemical constituents offer a versatile platform for designing materials with advanced and tunable functionalities. In particular, the integration of different metal–organic frameworks (MOFs) including or not functional bioentities enables the creation of complex hybrid porous systems with enhanced physicochemical, catalytic and biological properties.
Here we present recent advances in the engineering of MOF-based hybrid nanostructures through the controlled assembly of functional components, including MOF-on-MOF heterostructures and MOF-bioentities. Emphasis is placed on synthetic strategies that provide precise control over size, morphology, composition, and interfacial architecture, allowing the rational tuning of material performance. We further discuss how optimized interfacial interactions within these hybrids can significantly improve catalytic efficiency,[1,2] biological activity.[3]
These findings demonstrate the potential of framework diversification and hierarchical organization to unlock novel properties in MOF nanohybrids, advancing applications in enzymatic catalysis, polymer depolymerization, and biomedicine.

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S - D3 - 1F
Spray-made multifunctional, porous, and hybrid catalysts for sustainable chemistry

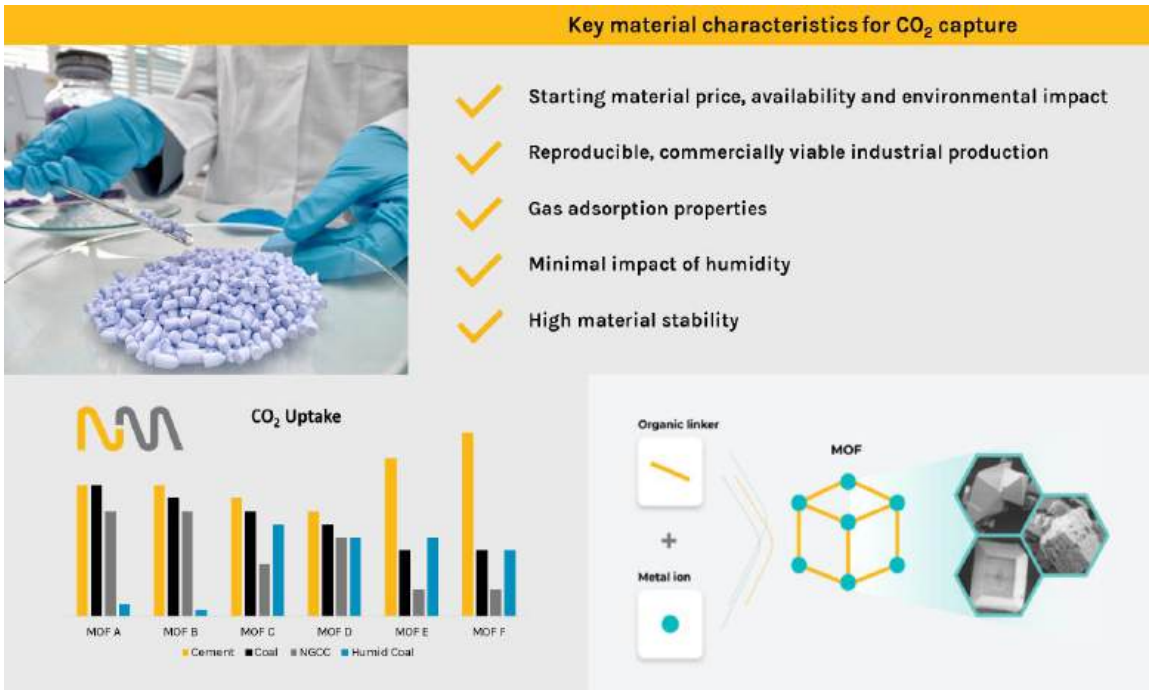
Damien P. Debecker
UCLouvain, Institute of Condensed Matter and Nanosciences (IMCN), Louvain-la-Neuve, Belgium

Heterogeneous catalysis relies on our ability to design, optimize, stabilize, and combine nanometric entities (metal nanoparticles, oxide clusters, enzymes, organic functionalities) at the surface of solid materials. Here, we will highlight the development of aerosol processes that are alluring for the continuous, scalable, and tailored production of advanced heterogeneous catalysts. Beyond the typical drying and aggregation of preformed particles via spray drying (or atomization), *reactive* aerosol processes allow *synthesizing* the materials in a bottom-up fashion, with tunable surface properties, textures, compositions, surface functionalities, etc. Inorganic polycondensation reactions and evaporation-induced self-assembly processes happen in seconds, confined in liquid droplets which act as “dynamic microreactors”. This peculiar mode of preparation has led to solid catalysts showing high performance in various applications including olefin metathesis, glycerol upgrading, olefin epoxidation, CO_2 hydrogenation, bio-alcohol dehydrogenation and dehydration, and even for the chemo-enzymatic synthesis of valuable chiral molecules.

S - D3 - 1G
Scaling carbon capture: Integrating tailored MOFs into industrial systems

K. Everden[1], C.Toft[1], A. Chomiak[1]
[1]novoMOF AG, Zofingen, Switzerland

The 2025 Nobel Prize in Chemistry was recently awarded for the development of Metal-Organic Frameworks (MOFs), which have demonstrated proven efficacy in various applications including CO_2 capture. As Metal-Organic Frameworks (MOFs) transition from laboratory-scale to pilot-scale demonstrators in sectors such as cement, steel, and power generation, their structural versatility offers a transformative alternative to conventional CO_2 capture technologies. However, the inherent variability of industrial process conditions, characterized by differences in temperatures, pressures, and moisture levels, precludes the existence of a "universal" MOF sorbent. This work provides an evaluation of state-of-the-art MOFs under a broad range of industrially relevant parameters, integrating material performance benchmarks with practical scale-up feasibility and shaping strategies. By clarifying the critical trade-offs between intrinsic material properties and macroscopic process design, we establish a strategic roadmap for tailoring MOF selection to specific industrial use-cases, ultimately accelerating their trajectory towards real-world deployment.



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S - D3 - 2
Embedding risk-based safety into chemistry education: A transatlantic dialogue

The purpose of this workshop is to foster a transatlantic dialogue that clarifies shared challenges, highlights emerging innovations, and identifies transferable principles for embedding risk-based safety thinking into chemistry education and research training across the EuChemS community.
Developing chemists who can think and act through a risk-based lens is an increasing priority in European and international contexts. Yet the ways in which safety is introduced, taught, and reinforced vary widely across institutions and regulatory environments. This two-hour interactive workshop brings together the EuChemS education and safety communities with representatives of the American Chemical Society (ACS) to examine how risk-based safety competencies can be embedded more intentionally across the chemistry curriculum.
The workshop presents the ACS's development of a RAMP framework (Recognize, Assess, Minimize, Prepare) into a scientific competency. The session does not present the ACS approach as a model to adopt, but as a framework that invites comparison with European practices.
A moderated dialogue invites participants to share how chemical safety is introduced in their own institutions; where responsibility for safety education sits; whether safety is taught explicitly, implicitly, or assumed; and what barriers or innovations they observe. These questions create a shared evidence-seeking space for European perspectives.
The workshop concludes by highlighting open-access educational safety resources that support cultural change and empower faculty.

S - D4 - 1
Natural polymers as the 21st century materials – From discovery to deployment

Material innovation is difficult and requires the alignment of enabling science and technology, critical scale and customers that take risks jointly to go from discovery to commercialization. At the forefront of these innovations are natural polymers that can be obtained from renewable feedstocks using chemical and biotechnological processes. While consumers are beginning to embrace sustainable materials as a gateway to circularity, there is no tolerance for a decrease in performance and their regulatory compliance compared to incumbent, synthetic materials such as plastics, which have experienced technological commercial growth of in the 20th century, but today face significant challenges with its end-of-life pollution to the environment. To that end, the industry-led ACS Green Chemistry Institute Natural Polymers Consortium aims to catalyze the sustainable development, production, and application of natural polymers in material science, and the foundational science that drives the acceptance and inclusion in policy and regulatory processes. This symposium will feature presentations from organizations leading Europe's efforts to foster collaborations, create synergies, and secure funding that are essential to accelerating the discovery, mass production and deployment of natural polymers as the 21st-century material in high-performance supply chains.

Schedule

10:00 - 10:05	Opening Remarks
10:05 - 10:20	Erlantz Lizundia (University of the Basque Country)
10:20 - 10:35	Jean-Marie Raquez (University of Mons)
10:35 - 10:50	Audrey Moores (McGill University)
10:50 - 11:05	Sergio Carballo (IFF)
11:05 - 11:20	Sander Defruyt (The Ellen MacArthur Foundation)
11:20 - 11:30	Edmond Lam (ACS Green Chemistry Institute)
11:30 - 12:00	Panel Discussion, Open Q&A, Closing Remarks

S - D4 - 1A

Natural polymers as potentially sustainable 21st century materials: Insights from lab-development and life cycle assessment

Erlantz Lizundia[1]

[1]*Life Cycle Thinking Group, Dept. of Graphic Design and Engineering Projects, Faculty of Engineering in Bilbao, University of the Basque Country (UPV/EHU), Bilbao, Spain*

Polymers from natural origin are abundant and renewable sources of carbon with a huge potential to be exploited as platform materials for multifunctional materials to rival those derived from fossil carbon. In this talk, we will explore how we can phase out of non-renewable, polluting resources and replacing them with biological, renewable alternatives. We will explore the use of these materials to preserve the current heritage, both natural and cultural heritage.

Here we exploit the processing versatility of these biopolymers, cellulose, chitin, chitosan and wood-derived materials mostly, to develop films and gels (using both top-down and bottom-up approaches) that can remove emerging contaminants from water, or to apply them in the conservation of cultural heritage artefacts.

We develop chitosan gels that show per- and polyfluoroalkyl substances (PFASs) removal capacities of 451 mg/g.[1] When combined with metal organic frameworks (MOFs), outstanding capacities reaching 690 mg/g could be attained, where a selective adsorption of carboxylate-terminated PFAS over sulfonates is observed. MOF incorporation markedly enhances the performance at a low carbon footprint increase, which in turn results in materials with improved performance-sustainability trade-off. We also develop a highly efficient capturing material derived from surface-modified wood to remove a broad spectrum of multidimensional and compositional micro and nanoplastics from water.[2] Chitinuous gels can remove salt efflorescence from bricks, both on the surface and inside the tested ancient mud-bricks, and are also efficient in cleaning antique ceramics.[3] We utilized life cycle assessment (LCA) to challenge the assumption that these natural materials present a low footprint per se. In addition, emerging modeling such as dynamic carbon accounting is utilized to get a more accurate picture of the actual physical climate change process related to bioproduct fabrication and utilization.[4]

This project has received a research grant from the UPV/EHU-AMVISA Water Classroom.

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S - D4 - 1B

Beyond valorization: Integrating biomass, sustainability, and knowledge systems for 21st century materials

Audrey Moores
Dept. of Chemistry, McGill University, Montréal, Canada; Stockholm University Center for Circular and Sustainable Systems (SUCCeSS), Stockholm University, Stockholm, Sweden

Biomass valorization is at the forefront of green and sustainable chemistry research. The use of renewable feedstocks is one of the twelve principles of green chemistry. Yet, the deployment of biomass-based technologies is inseparable from land use dynamics, ecological stewardship, and broader socio environmental systems. As sustainability imperatives intensify, these interconnections must be thoughtfully integrated into both research design and technological implementation.

In this presentation, I will introduce some of these concepts and propose the use of biomass waste as a potential avenue. I will highlight recent advances in the mechanochemical and aging mediated valorization of crustacean derived biomass waste into biopolymers,[1-3] functionalized biopolymer derivatives,[4-6] and nanostructured materials.[7-9] These strategies offer energy efficient pathways and reduced chemical and water inputs compared to conventional processing, demonstrating their promise for scalable and environmentally responsible manufacturing. Beyond technical innovation, the talk will also engage with broader perspectives from ongoing work that maps Indigenous knowledge systems onto contemporary sustainability research.[10] These perspectives offer critical insights into resource stewardship, circularity, and relational approaches to materials and environments.

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S - D4 - 1C

ACS Green Chemistry Institute Natural Polymer Consortium: Advancing the industrialization and commercialization of natural polymers

Edmond Lam[1], Isamir Martinez[1], Jun Wang[2], Matt Wagner[3]
[1]American Chemical Society, Green Chemistry Institute, Washington, DC, USA; [2]Colgate-Palmolive Company, Piscataway, NJ, USA; [3]The Procter & Gamble Company, Cincinnati, OH, USA

Natural polymers have the potential to sustainably meet today's consumer material needs as they are abundant and are part of circular carbon loop. There is potential to utilize the scientific knowledge gained from the efforts and resources already spent on petroleum-based plastic research and apply them to natural polymers. However, addressing the performance, processability, and high cost of translating natural polymer innovations to market-ready products requires broad multidisciplinary collaborations. Therefore, the American Chemical Society Green Chemistry Institute Natural Polymers Consortium (ACS NPC GCI) was formed to integrate the efforts from industry, academia, and other stakeholders to promote transformative research and application innovations for the industrialization and commercialization of natural polymers. This talk will present an overview of the strategic priorities of the industry-led ACS GCI NPC as it aims to catalyze the sustainable development, production, and application of natural polymers in material science. Key research priorities to address issues across the value chain important for accelerating the industrialization and commercialization of natural polymers will be described.[1]

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S - D4 - 1D

Designing next-generation bio-based polyhydroxyurethane nanocomposites with polysaccharide nanoreinforcements

Pavithra Wijeratne[1,2], Li Zha[2], Connie Ocando[1], Lars Berglund[2], Jean-Marie Raquez[1], Qi Zhou[2]
[1]Division of Glycoscience, Dept. of Chemistry, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH Royal Institute of Technology, AlbaNova University Centre,;Stockholm, Sweden; [2]Laboratory of Polymeric and Composite Materials, Dept. of Chemistry, Faculty of Science, University of Mons, Belgium

The transition toward sustainable polymers requires alternatives to conventional isocyanate-based polyurethanes that retain performance while reducing environmental and health concerns. Polyhydroxyurethanes (PHUs), synthesized via cyclic carbonate aminolysis, represent a promising isocyanate-free polyurethane platform[1], but their development has so far been limited by relatively low mechanical performance and challenges in processing[2]. This work addresses these challenges by developing bio-based PHU nanocomposites reinforced with polysaccharide-derived nanomaterials, focusing in particular on interfacial interactions, nanofiller structure, and processing methods. By deepening the understanding of structure–processing–property relationships in PHU-based biocomposites incorporating cellulose and chitin nanomaterials[3], a pathway for innovation is established that combines high performance with sustainability. The approach exemplifies how targeted chemical design, selection of renewable raw materials, and optimization for end-of-life considerations can together enable next-generation polymer composites that meet both technical demands and environmental imperatives.

Acknowledgements: This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement no. 955700. J.M.R is a FRS-FNRS Research Director and a WEL-T principal investigator from the WEL-T platform.

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S - D4 - 1E

Could natural polymers enable high-performing, recyclable and biodegradable paper-based flexible packaging and help address a major source of plastic pollution?

Sander Defruyt
The Ellen MacArthur Foundation, Belgium

Flexible packaging, like sachets, wrappers, and pouches, is a fast-growing plastic type, valued for being lightweight, functional, and low-cost. With low recycling rates and high rates of leakage into the environment in geographies lacking formal collection, it is also one of the hardest types to manage from a circularity and pollution perspective. Overcoming this systemic barrier would stop one of the largest sources of plastic packaging pollution.

A recent report by the Ellen MacArthur Foundation explores how paper-based alternatives could be one part of the solution, helping to reduce flexible packaging waste and pollution, especially in markets with high leakage rates.[1]

The report defines six critical criteria to ensure paper-based solutions are responsibly designed and deployed and support a circular economy - including being both recyclable and biodegradable. It is endorsed by more than 45 leading organisations and experts.

Given paper-based solutions that are both recyclable and biodegradable do not yet exist at the performance, scale and cost required, the report called for accelerated innovation for such solutions.

Crucial areas of innovation include high-performing, biodegradable coating materials, adhesives, and inks, as well as sustainably sourced, non-wood fibres. Could natural polymers play a role?

This presentation would invite the audience to get in touch with thoughts on the following questions:

- What is the potential for natural polymers to deliver high-performing paper-based packaging?
- How could innovation and scaling of natural polymers benefit from the strong demand for biodegradable paper-based packaging solutions?
- What could be the role of natural polymers in providing sustainable, non-wood fibres for paper?
- Is there a future for natural-polymer-based packaging (not paper-based)? How would you envision the end-of-life outcomes for these?

[1]Paper based flexible packaging – the role it could play in tackling small-format flexible plastic pollution in markets with high leakage rates. The Ellen MacArthur Foundation. **2026**. https://www.ellenmacarthurfoundation.org/paper-as-a-solution-to-flexible-packaging-pollution

S - D4 - 1F

Designed Enzymatic Biomaterials (DEB™) a versatile technology capable of providing functional performance coupled with advanced renewable carbon

Jure Zlopasa[1]
[1]*IFF, Oegstgeest, The Netherlands*

Polysaccharides are a class of biobased polymers that deserve a renewed focus given their large design space and rich functionality combined with intrinsic sustainability. Yet, being mostly extracted from plant based feedstock, current industrial polysaccharides such as cellulose and starch lack the intrinsic purity and molecular design precision found in synthetic polymers. Alternatively enzymatic polymerization of polysaccharides is one technology that can address some of the current limitations, allowing synthetic polymerization approaches. DEB technology enables polysaccharide development with a higher purity and polymer structure precision as well as the synthesis of hard to extract polysaccharides such as alpha-1,3-glucans. Moreover, the bottom-up assembly of insoluble polysaccharide polymers from soluble monomers allows the design of novel and rich colloidal features which, in turn, enable many industrial applications.
Sustainability continues to be a key driver for innovative product differentiation. Corporations around the world are setting specific sustainability metrics on new products. With a renewed emphasis on high performance biobased polymeric materials with the intrinsic design flexibility, DEB is offering functional performance to support novel solutions across a range of applications including coatings, flexible packaging, agriculture and fibers.

MS - D1 - 1A
Advanced non-target screening of environmental contaminants by high-resolution mass spectrometry

Chairs: Ester Heath, Adrian Covaci

Considerable progress in analytical instrumentation, informatics, and related fields has delivered powerful tools and techniques in environmental analysis for assessing chemical contamination. Among them, mass spectrometry (MS) has gained tremendous popularity thanks to its advantages, including unparalleled sensitivity and specificity, high resolution and wide dynamic range.
High-resolution mass spectrometry (HRMS) enables rapid detection and reliable identification of a range of contaminants, even in complex environmental matrices, thanks to full scan acquisition mode with high mass resolving power and high mass accuracy combined with advanced workflows for data prioritization and analysis. Screening techniques can either target the detection of several classes of known (suspect) compounds or employ a non-targeted approach using HRMS, which allows for the identification of otherwise unknown compounds through retrospective data analysis. In this regard, the use of HRMS-based approaches is changing the way we approach emerging contaminant research.
This mini-symposium disseminates the latest developments, challenges and opportunities in HRMS screening and data evaluation approaches with a focus on research involving environmental matrices (water, soil, indoor dust) and emerging contaminants, including per- and polyfluoroalkyl substances (PFAS) and plasticizers.

Presenters

12.45 - 13.00 **Xenia Trier** – Identifying volatile PFAS by GC-HRMS, for use in decision making
13.00 - 13.15 **Christian Zwiener** – Lessons learned from Nontarget Screening of contaminated sites
13.15 - 13.30 **Lidia Belova** – Ion mobility high-resolution mass spectrometry (IM-HRMS) for the characterization of phthalate homologue series in environmental samples
13.30 - 13.45 **Silvia Lacorte** – Non-targeted Gas Chromatography - Orbitrap Mass Spectrometry analysis of organic contaminants in certified reference materials

MS - D1 - 1B
Identifying volatile PFAS by GC-HRMS, for use in decision making

Xenia Trier
Dept. of Plant and Environmental Sciences, University of Copenhagen, Frederiksberg C, DK

With over 350,000 chemicals in use and numerous unknown transformation products, chemical pollution and its risks are likely underestimated. Non-target screening (NTS) by high-resolution mass spectrometry (HRMS) is increasingly used to identify chemicals of emerging concern. However, identification of volatile and neutral PFAS by GC-EI-HRMS is hampered by low molecular-ion abundance and the lack of reference standards, spectral libraries, and retention indices. This talk highlights recent methodological advances to enhance diagnostic ions through reduced fragmentation, increased injected mass, and prediction tools, and questions which identification level could be used in the future for regulatory decision making.

MS - D1 - 1C
Lessons learned from nontarget screening of contaminated sites

Christian Zwiener[1], Catharina Capitain[1], Melanie Schüßler[1]
[1]Eberhard Karls Universität Tübingen, Environmental Analytical Chemistry, Tübingen, DE

The total number of PFAS ranges from thousands to millions depending on the definition and source of information. Target analytical methods typically detect and quantify in most cases only much less than 100 PFAS. Therefore, nontarget screening (NTS) approaches are highly attractive for a more comprehensive characterization of PFAS contamination of humans, food, drinking water and the environment, which is important for risk assessment and mitigation. NTS approaches require suitable workflows with several steps of peak finding, blank correction, data reduction and prioritization before identification can be successfully performed.
In this work we present implications of our recent work on NTS for PFAS. This includes crucial steps in NTS measurements and data analysis workflows and the importance of NTS results for further assessment and mitigation measures. In a first example at an AFFF contaminated soil site, we demonstrate the importance of mass (m) and mass defects (MD) normalized to the carbon number (MD/C vs. m/C – plots) for prioritizing NTS data with high efficiency and subsequent successful tentative identification of 124 PFAS. The second example reveals the conclusions of a semi-quantification method based on matrix-matched average calibration curves for specific functional groups of PFAS and the consequences for site characterization and remediation measures. The third example demonstrates the use of NTS and identification of products of incomplete destruction to assess possibilities and limits of thermal treatment of AFFF contaminated soils. These examples underscore the importance of characterizing contamination as thoroughly as possible in order to conduct a meaningful assessment and plan effective mitigation measures.

We acknowledge BMFTR (Federal Ministry for Research, Technology and Space) for funding of the project PFClean (02WGW1665C).

MS - D1 - 1D

Ion mobility high-resolution mass spectrometry (IM-HRMS) for the characterization of phthalate homologue series in environmental samples

Lidia Belova[1], Maosen Zhao[1], Mikel Musatadi[1,2], Maarten Roggeman[1], Giulia Poma[1], Fatima den Ouden[1], Aline Murawski[3], Holger Koch[4], Alexander L.N. van Nuijs[1], Adrian Covaci[1]

[1]Toxicological Center, University of Antwerp, Antwerp, BE; [2]Dept. of Analytical Chemistry, University of the Basque Country (UPV/EHU), Leioa, ES; [3]German Environment Agency, Berlin, DE; [4]Institute for Prevention and Occupational Medicine of the German Social Accident Insurance, Bochum, DE

Ion mobility high-resolution mass spectrometry (IM-HRMS), an advanced separation technique, allows the separation of ions based on shape and size, providing an additional separation dimension. From measured mobilities, collision cross section (CCS) values are calculated providing an additional identification parameter in HRMS-based suspect screening, in particular for contaminant classes occurring in homologue series. These show characteristic relationships between CCS and *m*/*z* ratios described by class-specific CCS-*m/z* trendlines. While the use of these trendlines for compound annotation has been documented for per- and polyfluoroalkyl substances (PFAS)[1], their applicability for the annotation of other chemical classes remains largely unexplored.

This study focused on >40 indoor dust samples collected from private houses, kindergartens, public buildings in Germany and Belgium. After analysis by LC-IM-HRMS, data were matched with a suspect list containing > 4000 compounds, covering various classes of indoor contaminants. Despite the increasing use of alternative non-phthalate plasticizers, phthalates remained one of the major annotated classes with highest detection frequencies and semi-quantified concentrations[2]. Alongside legacy phthalates identified at confidence level (CL)1[3], annotated suspect phthalates covered two major classes: dialkyl and benzyl alkyl phthalates. Dialkyl phthalates included seventeen homologues with side chains ranging between C_1 (dimethyl phthalate) and C_{12} (didodecyl phthalate). Benzyl alkyl phthalates showed homologue series with alkyl side chain lengths between C_1 and C_{13}, vastly expanding on currently knowledge on this homologue series. Nevertheless, compound annotations were hampered by isomeric structures for each homologue, from differently branched side chains, leading to CL3 annotation. Obtained CCS values were used to describe the corresponding CCS-m/z trendline. Additionally, the use of high-resolution demultiplexing for post-acquisition increase of resolving power[4], allowed separating differently branched isomers. The experimental CCS values fell within the 90th percent confidence interval calculated for the CCS-m/z trendline deriving from available reference standards, contributing significantly to the confidence of the compound annotation.

[1]Dodds et al. **2020**; *Anal Chem*. 92(6): 4427-4435.
[2]Belova et al. **2024**; *Env Pol*. 345: 123475.
[3]Schymanski et al. 2014; *Environ Sci Technol.* 48(4): 2097-2098.
[4]Butler et al. **2022**; Anal Chem. 94(16): 6191-6199.

MS - D1 - 1E

Non-targeted gas chromatography - Orbitrap mass spectrometry analysis of organic contaminants in certified reference materials

Silvia Lacorte, Aina Queral, Ana Torres, Romà Tauler
Institute of Environmental Assessment and Water Research of the Spanish Research Council (IDAEA-CSIC), Jordi Girona, Barcelona, ES

Gas chromatography coupled to Orbitrap-mass spectrometry allows the low level and precise determination of organic contaminants in environmental samples. In this presentation, the target and untargeted performance of GC-Orbitrap-MS using the Regions of Interest Multivariate Curve Resolution (ROIMCR) and MSident chemical identification will be described. The applicability of such procedure will be demonstrated for the characterization of pollutants in certified reference materials: SRM 2585 (NIST) dust and ERM®-CE100 fish-based.

Acknowledgments: The Spanish Ministry of Science and Innovation is acknowledged for financial support with the project CHEMBIOPOL (PID2022-137766NB-I00).

MS - D1 - 2A
Society publishing with Chemistry Europe

Dr. Haymo Ross, Editor-in-Chief of *Chemistry - A European Journal*
Dr. Anne Nijs, Editor-in-Chief of the *European Journal of Organic Chemistry* and Managing Editor of *ChemistyrEurope*

Founded in 1995, **Chemistry Europe** is an association of 16 chemical societies that are members of EuChemS. The **mission** of the Chemistry Europe association is to evaluate, publish, disseminate, and amplify the scientific excellence of chemistry researchers from around the globe through high-quality publications. It publishes a family of high-quality scholarly chemistry journals covering a very broad range of chemistry disciplines, including the namesake flagship open access journal *ChemistryEurope*, which will be featured in the talk.

MS - D2 - 1A

Modernizing chemistry education for new challenges and responsibilities: RDM & data science in the curriculum

Hans-Georg Weinig[1],Jochen Ortmeyer[2]
[1]Chair ECTN Workgroup Core Chemistry, German Chemical Society GDCh, Frankfurt am Main, Germany;
[2]NFDI4Chem, RWTH Aachen, Germany

The mini-symposium will include 3-4 short presentations and address how Bachelor-level chemistry education must evolve to prepare graduates for a data-intensive, digitally networked research landscape. Building on the European Chemistry Thematic Network's[1] (ECTN) recently updated recommendations for bachelor-level chemistry programmes (Core Chemistry) and leveraging community infrastructures such as NFDI4Chem[2] and the Physical Sciences Data Infrastructure[3] (PSDI), it focuses on embedding research data management (RDM), data science and open science as transversal elements of the curriculum.
Rather than adding disconnected "digital" modules, the symposium will explore how good RDM practices and basic data-science competencies can be integrated into the existing core chemistry content and laboratory courses. NFDI4Chem's discipline-specific guidelines on FAIR (Findable, Accessible, Interoperable, Reusable) data, electronic lab notebooks, metadata, persistent identifiers and reproducible workflows will provide a reference for turning traditional lab documentation into structured, machine-actionable records. In parallel, PSDI's cross-domain perspective will highlight interoperable infrastructures and services that enable the long-term reuse and linking of chemical data across the physical sciences.
By bringing together curriculum developers, infrastructure initiatives and educators, the mini-symposium aims to formulate concrete, implementable recommendations for modernizing European chemistry programmes. The goal is to empower future chemists to assume their emerging responsibilities as competent data producers, managers and users, strengthening both scientific quality and societal trust in chemical research.

[1]https://ectn.eu/
[2]https://nfdi4chem.de/
[3]https://www.psdi.ac.uk/

MS - D2 - 2
Zoo science for conservation

Herwig Leirs[1,2]
[1]University of Antwerp, Belgium; [2]Royal Antwerp Zoo Foundation, Belgium

The congress venue belongs to the Royal Antwerp Zoo Foundation. When that organization was founded in 1843, its mission was to show exotic animals as an (educational) pass-time for the Antwerp upper class in what was then a rural area outside the city walls. Since then millions of guests have visited the currently two zoos, one in Antwerp, the other one near Mechelen. Over the years the mission of zoos has changed considerably. While a zoo still needs to remain attractive for visitors, the collection of animals is nowadays less determined by what the public wants to see, but by the need to maintain species for which zoo populations may be important rescue sources, and to keep them in a way that allows as much as possible their natural behaviour. This obviously comes with specific challenges about housing, management, genetics etc.
The Royal Antwerp Zoo Foundation emphasizes the role of science as a basis for biodiversity conservation. The main research themes of its Center for Research and Conservation are (i) Animal welfare and health, (ii) Population management, (iii) Nature conservation and restoration and (iv) Animal behaviour, evolution and cognition. During this presentation, I will present several studies illustrating this research diversity.
Research and conservation not only happen *ex situ* (in captivity) but also *in situ* (in the wild). Currently the majority of the efforts of the Antwerp Zoo Foundation go to lowland forests on the left and right bank of Congo River in DRC where resp. populations of bonobos and okapis are supported and studied, to mixed cacao plantation landscapes with golden-headed lion tamarins in Brasil, the brown vulture reintroduction program in S.Europa and the large peatland reserve "De Zegge" in Flanders. In all those places, involving surrounding communities is a core aspect of the conservation plans. Obviously there will be time for questions and discussions.

MS - D2 - 3
PFAS (per- and polyfluoroalkyl substances)

Prof. Dr. Christian Zwiener - Session chair
University of Tübingen, Germany

PFAS comprise more than 10,000 individual compounds used in a broad range of applications (industry, firefighting foams, consumer products) and are found globally in water, soil, plants, animals, and also in remote areas due to atmospheric transport. Health concerns arise from their toxicity (cancers, immune issues, developmental problems), very high stability, environmental persistence and accumulation in living organisms. Challenges arise from the still considerable knowledge gaps about the sources, identity and fate in environment and biota of individual PFAS, as well as from the insufficient coverage of PFAS by target analytical methods. Biotic and abiotic transformation processes of polyfluorinated compounds, so-called precursors, complicate the matter further. Therefore, new analytical approaches like nontarget screening or sum parameters for organic fluorine are required. This symposium sets some spotlights on different aspects of PFAS including advanced analytical methods for identification and passive sampling, occurrence and fate of PFAS during long-range transport and in agricultural soils.

Tue, July 14, 12:45 – 13:45 hrs

12:45 – 12:55	**Introduction to the challenge of PFAS** C. Zwiener, Tübingen, DE
12:55 – 13:10	**Ion-mobility derived CCS-m/z trendlines for improved annotation confidence of PFAS** A. Covaci, Wilrijk, BE
13:10 – 13:25	**Ceramic assive approaches to determine PFAS in water** S. Lacorte, Barcelona, ES
13:25 – 13:40	**Long-range atmospheric transport potential of perfluorocarboxylic acids** G. Lammel, Mainz, DE
13:40 – 13:55	**Fluorinated compounds in agricultural formulations used in rice cultivation** B. Oró-Nolla, Tübingen, DE
13:55	**Wrap up and final discussion**

MS - D2 - 3A Ion-mobility derived CCS-*m*/*z* trendlines for improved annotation confidence of PFAS

Adrian Covaci[1], Lu Zhao[1,2], Oliver Salangad[1], Francesca Cappelli[1], Jodie Buytaert[3], Thimo Groffen[3], Lieven Bervoets[3], Lidia Belova[1]
[1]*Toxicological Centre, University of Antwerp, Belgium*
[2]*Interdisciplinary Research Academy, Zhejiang Shuren University, China*
[3]*ECOSPHERE, University of Antwerp, Antwerp, Belgium*

Collision cross section (CCS) values derived from ion mobility high-resolution mass spectrometry (IM-HRMS) can serve as an additional identification parameter in suspect and non-target screening analyses of contaminants of emerging concern (CECs). The use of CCS data usually relies on the comparison of experimental datapoints with library values. As the current online libraries often lack values for newly identified CECs, CCS prediction tools can provide artificial reference data. However, the prediction of CCS values for (classes of) compounds not included in the data used to train the prediction models can lead to high deviations (up to 10%) compared to experimental CCS values derived from analysis of reference standards[1]. We present the advantages of using CCS-*m*/*z* trendlines (i.e., the relationship between CCS values and mass-to-charge (*m*/*z*) ratios) for the annotation of suspect per- and polyfluoroalkyl substances (PFAS).
In this study, PFAS were investigated by LC-IM-HRMS in eggs (n=41) of the passerine birds great and blue tits and soils collected in the vicinity of a PFAS-producing plant in Antwerp (Belgium). Due to their unique structure, which typically includes linear and branched alkyl chains and functional groups, most PFAS compounds exist as isomers. Based on the available standards for PFOS isomers (11) and the CCS values obtained from other PFAS, we detected several branched isomers of PFBS (2), PFHxS (6), PFOS (7), PFNS (2), PFDS (5), PFDoS (11), PFOA (10), PFNA (6), PFDoDA (1), PFTrDA (3), and FOSA (1), for which analytical standards were not available. A significant difference in the distribution of PFOS isomers between the two bird species' eggs was observed, which may be related to variations in lifespan and foraging habits. The results demonstrate that LC-IM-HRMS is a useful tool for the analysis and identification of branched PFAS isomers, particularly in the absence of reference standards.

Reference:
[1] Belova, L., Celma, A., et al., Anal Chim Acta, **2022**; 1229: 340361.

MS - D2 - 3B Ceramic Passive approaches to determine PFAS in water

Silvia Lacorte
Institute of Environmental Assessment and Water Research of the Spanish Research Council (IDAEA-CSIC), Jordi Girona, Barcelona, Spain

Passive Sampling is emerging as a new procedure for monitoring water contaminants in a precise and representative manner. Among other contaminants, perfluoroalkyl and polyfluoroalkyl substances (PFAS) are of concern due to their widespread presence in waters, persistence and effects they may cause on aquatic organisms. This presentation discusses the use of ceramic passive samplers (CPS) and other passive samplers (PS) to detect multiple PFAS in water. Challenges regarding PS calibration, deployment conditions, fouling and effect of water type will be described. In addition, the potential of non-target screening to increase the scope of PFAS identification in water will be explored. The final aim is to implement PS to allow a comprehensive screening of PFAS in several water types.

Acknowledgments
The Spanish Ministry of Science and Innovation is acknowledged for financial support with the project CHEMBIOPOL (PID2022-137766NB-I00).

MS - D2 - 3C Long-range atmospheric transport potential of perfluorocarboxylic acids

Gerhard Lammel[1,2], Karsten Baumann[1,3], Dominika Bezdeková[1], Jiři Kohoutek[1], Petra Přibylová[1], Üllar Rannik[5], Petr Šenk[1], Risto Taipale[6]
[1]Masaryk University, Faculty of Science, RECETOX, Brno, Czech Republic; [2]Max Planck Institute for Chemistry, Multiphase Chemistry Department, Mainz, Germany; [3]University of North Carolina, Gillings School for Global Public Health, Chapel Hill, USA; [4]University of Helsinki, Department of Physics, Helsinki, Finland; *[5]University of Helsinki, Institute for Atmospheric and Earth System Research, Helsinki, Finland*

Per- and polyfluorinated alkyl substances (PFAS) are globally distributed environmental pollutants, persistent, bioaccumulative, and toxic and a severe concern for ecosystems and human health.
Perfluorocarboxylic acids (PFCAs) are semivolatile substances which following atmospheric deposition may re-volatilise from surfaces. Atmospheric deposition is the main source for PFCAs in soil and surface waters. Because of their amphiphilic structure PFCAs are accumulated on water surfaces and in biofilms.
Recent trends of PFCA atmospheric distributions and air-surface exchanges will be presented, as well as modelling approaches to simulate and understand large-scale PFCA distributions and fate.

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MS - D2 - 3D Fluorinated compounds in agricultural formulations used in rice cultivation

B. Oró-Nolla[1,3], Maria Dulsat-Masvidal[2], A. López-Antía[3], S. Lacorte[3], C. Zwiener[1]
[1]Environmental Analytical Chemistry, Dep. of Geosciences, Universität Tübingen, Germany
[2]Ecology and Evolutionary Biology, Dep. of Biology, University of Turku, Finland
[3]Ch4EO, Dep. of Environmental Chemistry, IDAEA-CSIC, Barcelona, Catalonia, Spain

Birds are bioindicators of chemical pollution, and some species feeding in vulnerable habitats give information on perfluoroalkyl substances (PFAS) distribution and concentration levels. A recent study revealed the presence of perfluorooctanoic acid (PFOA), as the main compound, in blood of two-month-old flamingo chicks from the Ebro Delta at 38.5 ± 8.20 ng/mL in 2019 and at 12.2 ± 1.30 ng/mL in 2024, while other PFAS were detected in water samples (n=8), from 22.9 to 65.8 ng/L, with highest concentrations in agricultural fields. Fluorinated pesticides represent a rapidly expanding class of agrochemicals, yet their contribution to PFAS in agricultural environments is poorly understood and their impact on wildlife remains unknown.
Our hypothesis is that PFAS might come from pesticide formulations which are acting as diffuse sources of trifluoroacetic acid (TFA) and ultra-, short- and long-chain PFAS, either because of 1) the degradation of the active ingredients or 2) the presence of diverse fluorinated co-formulants. Here, we focused on the analysis of Novixid®, one of the most used products in the Ebro Delta rice fields. The Photocatalytic Total Oxidizable Precursor (PhotoTOP) assay [1] was used to identify degradation products coming from fluorinated active ingredients, and/or coming from additives. This formulation was extracted by solid phase extraction (SPE) and the elution was achieved with a C_{18} chromatographic column. Analyses were achieved by HPLC coupled to a quadrupole time-of-flight mass spectrometer (QTOF) in negative electrospray ionization mode (ESI −). Prioritization of features and identification of other potential PFAS was performed PFΔScreen [2] and the blanks, to remove background signals.
Results showed that for penoxsulam (10 ng/mL initial concentration), the active ingredient of Novixid containing a $–CF_3$ group, TFA was formed at a concentration of 0.73 ng/mL. PFOA and PFNA were also detected at 0.25 and 0.10 ng/mL, respectively, after the oxidation experiment, suggesting that they can occur as degradation products from still unknown precursors. For the SPE, a hydrogen-substituted perfluorodecanoic acid ($C_{10}H_2F_{18}O_2$) was identified as one of the main fluorinated compounds. With this approach, new chemicals will be identified as fluoropolymer additives, emulsifiers or transformation products coming from the pesticide formulations.

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EuChemS Division of Organic Chemistry Award Lectures

In this symposium:
Prof. Helma Wennemers (ETH Zürich) will receive the EuChemS Female Investigator Award;
Dr. Johannes Wahl (Uni Mainz) will receive the Young Investigator Award;
Prof. Pat Guiry (University College Dublin) will receive the Award for Service.

Both Prof. Wennemers and Dr Wahl will present their research.

MS - D2 - 4A
Asymmetric catalysis with peptides – From simple to complex environments

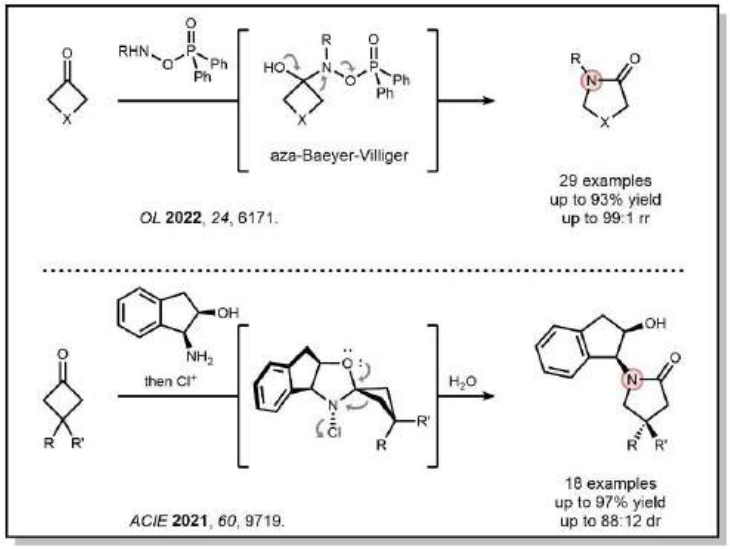
Helma Wennemers
Laboratory of Organic Chemistry, D-CHAB, ETH Zürich, Zürich, Switzerland

In nature, proteins fulfill manifold different functions and are crucial, for example, as enzymes or templates for the controlled formation of structural components such as bones. The Wennemers group is intrigued by the question of whether peptides with significantly lower molecular weights than proteins can fulfill functions for which nature evolved large macromolecules. Specifically, we ask whether peptides can serve as effective asymmetric catalysts, synthetic collagen-based materials, or imaging and targeting agents for fibrotic tissue.
The lecture will focus on stereoselective peptide catalysts of the general type H-Pro-Pro-Xaa. These peptides allow for catalysis *via* an enamine intermediate, with catalyst loadings of as little as 0.05 mol%, and provide synthetically versatile products from aldol and conjugate addition reactions with high stereoselectivities. The lecture will discuss the scope of the peptide-catalyzed reactions and insights into the mechanism. We will show which structural and functional features distinguish the peptides from other chiral amine catalysts and highlight how changes in the conformational properties enable tuning of the catalytic activity, stereoselectivity, and chemoselectivity. In addition, the lecture will present peptide catalysis in complex environments (e.g. cell lysates) and cascade reactions with enzymes.

MS - D2 - 4B
Molecular editing by nitrogen insertion

J.M. Wahl
Johannes Gutenberg-Universität, Mainz, Germany

Molecular editing describes the idea to change the skeleton of an advanced molecule in a mild and selective fashion. This concept has come to the forefront of organic chemistry because of its promising impact on medicinal chemistry. However, many simple transformations that allow the precise “editing” at the late stage of a synthetic sequence have not reached maturity yet. One example is the introduction of nitrogen, which is of great interest based on the high percentage of nitrogen atoms in current drug molecules. Within this talk, methods that allow the selective nitrogen insertion into strained rings will be presented.
In 2020, we engaged in the mechanistic elucidation of nitrogen insertions into cyclobutanones.[1] Based on our experimental results, a mechanistic pathway different from the classical Beckmann rearrangement was found. Within this aza-Baeyer-Villiger reaction paradigm, we developed exceptionally mild conditions by using amino phosphinates to ensure nitrogen insertion. Thus, a variety of γ-lactams became accessible.
A mostly unsolved problem is the enantioselective introduction of a nitrogen atom,[2] which prompted us to develop an asymmetric approach by mimicking the tetrahedral intermediate of the aza-Baeyer-Villiger reaction.[3] By using widely available aminoindanols, we completed the first highly selective nitrogen insertion towards γ-lactams via oxidation of the intermediary formed *N*,*O*-ketals. The applicability of the methods was showcased by the synthesis of the two drug molecules rolipram (anti-depressant) and brivaracetam (anti-epileptic). Building upon these initial results, we currently succeeded in a Brønsted acid catalyzed asymmetric nitrogen insertion[4] and at a variant for nitrile synthesis via ring contraction,[5] which will be covered within my talk.



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MS - D3 - 1
The new Intergovernmental Science-Policy Panel on Chemicals, Waste and Pollution (ISP-CWP)

Panel Discussion

20 June 2025 was a historic day, when the United Nations Environment Programme (UNEP) established the new Intergovernmental Science-Policy Panel on Chemicals, Waste and Pollution (ISP-CWP). https://www.unep.org/isp-cwp

The ISP-CWP will be a hugely important sister Panel to the Intergovernmental Platform on Biodiversity and Ecosystems Services (IPBES) and the Intergovernmental Panel on Climate Change (IPCC) to provide independent scientific evidence to help address the triple planetary crisis of climate change, biodiversity loss and pollution from chemicals and wastes. The ISP-CWP is now being set up and the rules of procedure, work programme and issues of concern being developed and agreed by governments.

This panel discussion at ECC10 will raise awareness and provide an update on the progress on the establishment of the ISP-CWP and begin to engage scientists who may wish to contribute to the work of the panel in the months and years ahead.

The success of the ISP-CWP is going to rely on engaging multidisciplinary expert scientists in its work, synthesising and reviewing technical evidence, and providing advice and making recommendations for possible solutions to chemicals, waste and pollution issues based on the latest state of the art evidence. This is an opportunity to explain and discuss why chemical scientists are going to be so important.

The Chair of this session will be Professor Tom Welton OBE, Ambassador in Sustainable Chemicals Policy at the Royal Society of Chemistry. Each panellist is asked to present their perspectives on the ISP-CWP in 5 minutes around key questions below, and then there will be an open discussion. There may be some time for a few questions or comments from the floor.

1) How can scientists become more involved in the work of the ISP-CWP and connect across to the Global Framework on Chemicals (GFC)?
2) How can scientific independence be built into the ISP-CWP?
3) How can the ISP-CWP ensure that it gets the advice that it needs from all disciplines?
4) If you could ask one question of the ISP-CWP to address first, what would it be?

Proposed panellists:

- **Tom Welton OBE** (Chair) – Emeritus Professor, Imperial College London.
- **Bart Rymen** – Vice Chair of the ISP-CWP - Attaché, Federal, Interfederal and International Coordination, Belgian Science Policy Office
- **Gabriel Sigmund** – Associate Professor, Wageningen University, The Netherlands.
- **Anna Isabel Becker** - Director of Policy, ISC3, Germany.
- **Matthew Davies** – UNESCO Chair, Professor at Swansea University, Wales.
- **Janna Radi** – Children & Youth Major Group representative, Cairo, Egypt.

Rare earths from e-waste: A sustainable path for energy and emerging technologies

Eduarda Pereira[1], Thainara Viana[2], Bruno Henriques[2]
[1]Central Laboratory of Analysis, University of Aveiro, Portugal; [2]LAQV-REQUIMTE – Associated Laboratory for Green Chemistry, Department of Chemistry, University of Aveiro, Portugal

The transition towards low-carbon energy systems and the rapid expansion of emerging technologies have led to an unprecedented increase in the demand for rare earth elements (REEs). These critical raw materials are indispensable for manufacturing high-performance permanent magnets, electric vehicles, wind turbines, electronic devices, and numerous advanced technologies. However, the limited geographical distribution of primary resources, increasing supply risks, and environmental concerns associated with conventional mining have intensified the search for sustainable alternative sources. Secondary resources, particularly electronic waste (e-waste) and mining-related residues, represent valuable reservoirs of REEs that can contribute to a more circular and resilient economy.

This minisymposium will present recent advances in the recovery of REEs from secondary resources, with a particular focus on environmentally friendly sorption-based approaches. An introductory presentation will provide an overview of the strategic importance of alternative REE sources within the context of the energy transition and emerging technologies, highlighting the role of resource recovery in securing future supply chains. Subsequent contributions will demonstrate the potential of sorption as a versatile and sustainable methodology for REE recovery from complex multi-element solutions. Case studies will include the use of bio-based sorbents and synthetic materials for the selective recovery of REEs from leachates generated from end-of-life wind turbine components[1], illustrating the challenges and opportunities associated with complex waste streams. The symposium will also showcase innovative research on the recovery of REEs from acid mine drainage using living macroalgae[2], highlighting the potential of biological systems as low-impact technologies for metal recovery and environmental remediation, as illustrated by Figure 1.

By bringing together complementary perspectives on sustainable REE recovery, this minisymposium aims to foster interdisciplinary discussion on innovative separation technologies, valorisation of secondary resources, and circular economy strategies. It will provide a platform for researchers to discuss recent advances and future directions towards securing critical raw materials for a sustainable energy future.

Fig. 1. Schematic illustration of the circularity of recovering rare earth elements from secondary sources using macroalgae.

This work is funded by COMPETE2030-FEDER-00847800 and national funds from FCT/MCTES through project UID/50006/2025 — Laboratório Associado para a Química Verde—Tecnologias e Processos Limpos. Thainara Viana thank FCT/MCTES for PhD grant ref. 2022.13015.BD.

[1]Ferreira, N.; Viana, T.; Nunes, C.; Pereira, E.; Henriques, B. “Optimising the selective recovery of rare earth elements from multi-element solutions using untreated shrimp shells”. *Process Safety and Environmental Protection*. **2026**, vol. 215, p. 109117.
[2]Viana, T.; Ferreira, N.; Pereira, E.; Henriques, B. “Seaweed as a sustainable solution for rare earth elements removal from acid mine drainage”. *Journal of Environmental Chemical Engineering*. **2025**, vol. 13, p. 116484.

MS - D3 - 3
New strategies for analytical chemistry in environmental assessments

Date: 15 July 2026 **Session:** 12:45 – 13:45 **Format:** 4 × 15-minute presentations

Time	Presenter	Title
12:45 – 13:00	**Roland Kallenborn**	*Future Analytical Methods for Screening of Chemicals of Emerging Arctic Concern (CEACs)*
13:00 – 13:15	**Jiri Barek**	*SWOT Analysis of Modern Trends in Electroanalytical Chemistry*
13:15 – 13:30	**Silvia Bruguera Lacorte**	*Ceramic passive samplers for pollutant monitoring*
13:30 – 13:45	**Ester Heath**	*Challenges and Opportunities for Sludge as Resource in Agricultural Applications*

MS - D3 - 3A
Future analytical methods for screening of Chemicals of Emerging Arctic Concern (CEACs)

Roland Kallenborn
Norwegian University of Life Science /NMBU)s, Faculty of Chemistry, Biotechnology and Food Sciences (KBM), Norway

The Arctic environment represents one of Earth's most pristine yet increasingly vulnerable ecosystems. Despite its remoteness, the Arctic serves as a terminal sink for persistent organic pollutants and emerging contaminants transported via long-range atmospheric and oceanic pathways. As regulatory frameworks evolve and industrial activity in polar regions expands, the identification and monitoring of Chemicals of Emerging Arctic Concern (CEACs) has become a scientific and environmental priority of urgent global relevance. Current analytical approaches, while robust for legacy pollutants, face significant limitations when applied to the complex and often structurally diverse landscape of CEACs — including per- and polyfluoroalkyl substances (PFAS), microplastic-associated chemicals, pharmaceutical residues, and novel flame retardants. Low ambient concentrations, matrix complexity from unique Arctic biota and cryospheric media, and the sheer number of uncharacterized compounds challenge conventional targeted monitoring strategies. This presentation outlines the trajectory of next-generation analytical methodologies poised to transform CEAC screening in Arctic matrices. Particular emphasis is placed on high-resolution mass spectrometry (HRMS) combined with suspect and non-target screening (NTS) workflows, enabling the simultaneous detection of thousands of chemical features without prior structural knowledge. Integration of machine-learning-assisted spectral annotation and open-access chemical databases substantially accelerates compound identification and prioritization. Furthermore, advances in miniaturized and field-deployable analytical platforms offer transformative potential for in situ Arctic monitoring, reducing logistical barriers inherent to remote sampling campaigns. Passive sampling technologies, coupled with multi-residue extraction protocols optimized for Arctic-specific matrices such as sea ice, snow, and Arctic marine organisms, are discussed as complementary approaches. Collectively, these methodological innovations represent a paradigm shift toward comprehensive, discovery-driven chemical surveillance, critical for safeguarding Arctic ecosystem integrity and informing evidence-based environmental policy at national and international levels.

MS - D3 - 3B
SWOT analysis of modern trends in electroanalytical chemistry

Jiri Barek
Charles University, Faculty of Science, Dept. of Analytical chemistry, UNESCO Laboratory of Environmental Electrochemistry, Prague, Czech Republic

The presentation will focus on possibilities and limitations of modern electroanalytical methods in the field of large scale high through put monitoring especially of biologically active organic compounds important from the point of view of environmental and human health protection[1]. Advantages and disadvantages of modern analytical methods will be evaluated using now popular SWOT analysis. The advantages connected with portability, sensitivity, selectivity, low cost, and compatibility with green and white analytical chemistry will be compared with disadvantages connected with problems with minimizing parts of curriculum vitae devoted do electroanalytical methods. Problems with accepting new electroanalytical methods in commercial laboratories, with introduction of novel electrode materials, eg. boron doped diamond[2], solid amalgam[3], various forms of carbon[4], etc. and with novel electrode arrangements, will be disused and evaluated.

Acknowledgements: This work was financially supported by the Grant Agency of the Czech Republic (project GAČR 25-16569S). Material, technical and intellectual support of Metrohm.CZ (www.metrohm.com/cs-cz/) is highly appreciated.

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[2]Augustín M.; Vyskocil V; Szabó O; Dragounová K.A.; Aubrechtova K.; Pfeifer R; Matysik F.M.; Barek J; et al. *Electrochim. Acta* **2025**, 514, 145549. https://doi.org/10.1016/j.electacta.2024.145549.
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MS - D3 - 3C
Ceramic passive samplers for pollutant monitoring

Silvia Lacorte, Ana Piera, Marta Herrero
Institute of Environmental Assessment and Water Research of the Spanish Research Council (IDAEA-CSIC), Barcelona, Spain

Passive sampling has emerged as a promising approach for monitoring aquatic contaminants by providing time-integrated and representative measurements of chemicals present in a water body. This study introduces the ceramic passive samplers (CPS) as a multi-contaminant monitoring device. CPS consist in a porous cylindrical ceramic membrane whose structure can be customized to facilitate the diffusion of dissolved contaminants at different rates, allowing its deployment in different types of water and during different periods of time. A sorbent housed within the internal compartment of the CPS enables the uptake of contaminants of different physico-chemical properties. In this presentation, different uses of CPS are demonstrated, including wastewater, river water and drinking water. Their ability to detect multiple contaminants with high sensitivity is demonstrated, highlighting the importance of implementing advanced monitoring strategies to safeguard both aquatic ecosystems and human health.

MS - D3 - 3D

Agricultural reuse of treated wastewater and sludge: Uptake of contaminants of emerging concern

E. Andreasidou[1,2], A. Kovačič[1,2], D. Heath[1], M. Pintar[3], N. Kacjan Maršič[3], U. Blaznik[4], A.R. Fernández-Alba[5], M.D. Hernando[6], E. Heath[1,2]

[1]Dept. of Environmental Sciences, Jožef Stefan Institute, Slovenia; [2]Jožef Stefan International Postgraduate School, Slovenia; [3]Dept. of Agronomy, Biotechnical Faculty, University of Ljubljana, Slovenia; [4]National Institute of Public Health, Environmental Health Centre, Slovenia; [5]Dept. of Chemistry and Physics, University of Almería, Spain; [6]Dept. of Desertification and Geo-ecology, Experimental Station of Arid Zones, CSIC, Spain

The reuse of treated wastewater (TWW) and sewage sludge in agriculture is increasingly promoted as a sustainable strategy to address water scarcity, nutrient recovery, and growing food demand. However, contaminants of emerging concern (CECs) may be present in TWW, accumulate in crops, and pose potential risks to food safety. This study investigated the uptake and translocation of 27 CECs in tomato plants in field (lysimeters) and pot experiments.

The field experiment evaluated irrigation with potable water, TWW, and the respective media spiked with CECs (1 mg/L). In tomatoes irrigated with TWW, only carbamazepine was above the limit of quantification (22 ng/g dry weight). In tomatoes irrigated with spiked media, six CECs were quantified (acetamiprid, azithromycin, BPS, carbamazepine, clarithromycin, and dimethomorph), while up to 17 CECs were present in roots>leaves>stems. Dietary exposure assessment indicated no acute health risk from TWW-irrigated tomatoes. Azithromycin and triclocarban were present in soil up to 30 months after irrigation and exceeded safety thresholds. The pot experiment included tomatoes grown in peat substrate amended with anaerobically digested (dried) sludge at two rates corresponding to nitrogen and nitrogen/potassium requirements. Additional treatments included CEC-spiked media and peat amended with non-dried sludge. In treatments without spiking, ibuprofen and triclosan were quantified in tomato fruits at the low amendment rate. At the high amendment rate, caffeine, carbamazepine, ciprofloxacin, and ibuprofen were quantified. Carbamazepine, the only compound detected in all plant tissues, showed the highest translocation from roots to leaves, followed by stems and fruits. Dietary exposure was below risk thresholds, except for BPS when non-dried sludge was applied. Environmental risk assessment indicated risk quotients >1 for seven CECs in sludge-treated systems. When comparing the two experiments, different CECs were present in tomato fruits, suggesting that bioaccumulation can depend on the source of CECs. Specifically, sludge amendment can enable the desorption of compounds into pore water, thereby increasing bioavailability. In contrast, the field's soil composition may lead to strong sorption. Overall, although limited risks were identified for consumers, both treated wastewater and sludge applications led to the accumulation of CECs in soil, an aspect that should be considered in repeated reuse applications.

MS - D4 - 1
On the impact of artificial intelligence in chemistry and beyond

Tom Børsen[1], Jan Mehlich[2], Anca Silvestru[3], Hans Steisslinger[4]
[1]Aalborg University, Denmark; [2]Rheinische Friedrich-Wilhelms-Universität Bonn, Germany; [3]Babeş-Bolyai University in Cluj Napoca, Romania, [4]Terra Institute, Germany

The workshop builds on the presentations delivered by members of the EuChemS Working Party on Ethics in Chemistry. Its aim is to provide a structured forum for collective reflection on how artificial intelligence is reshaping chemistry and its role in society. Particular attention is given to the societal and sustainability-related ethical challenges that accompany the increasing use of AI in chemical research, innovation, and practice.

The workshop is organised around two rounds of facilitated group discussions.

Round 1 (Thursday, 16th July 2026, morning session, 10.00 – 12.00)
The debate will be focused on the presentations RC-D4-I1, RC-D4-001, RC-D4-002, RC-D4-003.
Participants will discuss which ethical issues they consider most critical for chemistry and its practitioners from a societal perspective. These include, but are not limited to, chemistry's responsibility in relation to sustainable development, environmental and climate impacts, resources use, technological responsibility, inequalities in access to data and AI-enabled tools, and issues of research integrity, such as data quality, reproducibility, transparency, and accountability in scientific practice.

Round 2 (Thursday, 16th July 2026, afternoon session, 14.00 – 15.30)
The debate will be focused on the presentations RC-D4-006, RC-D4-007, as well as on the conclusions of the first round.
Participants will explore how artificial intelligence intersects with and influences the ethical challenges, based on specific examples. Discussions will address both AI's potential to accelerate scientific discovery and the green transition, and the risks associated with bias, lack of transparency, unintended consequences, and shifting responsibility in complex, AI-supported research and decision-making systems.
The second round of the workshop will conclude with a synthesis of the discussions, forming the basis for a report summarising key themes, perspectives, and recommendations. To encourage open and candid dialogue, the workshop will be conducted under the Chatham House Rule, meaning that participants are free to use the information received, but neither the identity nor the affiliation of speakers or other participants may be revealed.

MS - D4 - 2
Unlocking publication success: Your guide to publishing in Angewandte Chemie Journals

Dr. Charlotte Gers-Panther
Editor-in-Chief of *Angewandte Chemie Novit*

Angewandte Chemie is a household name in high-impact chemistry publishing, known for its rigorous editorial standards. Since 2025, the portfolio addition, *Angewandte Chemie Novit*, offers a new and unique route to publishing exceptional research – The Up-Transfer. We invite you to join this workshop, where you will gain insights into what the editors seek in a manuscript, learn about the thorough evaluation and selection processes for both journals, and discover practical strategies to help your research thrive within the Angewandte Chemie family. Whether you are an early-career scientist or a seasoned researcher, this session is designed to empower and inspire your journey toward publication success!

MS - D4 - 3

AI, reshaping chemistry education: Curriculum design, student skills, and departmental decision making

Veeran C.[1], Hilven L.[2], Evers C.[3]
[1]Pearson Higher Education, Munich, Germany; [2]Pearson Benelux, Belgium

Introduction: Digital learning platforms and AI-supported study tools are increasingly integrated into higher education chemistry curricula. Institutions are seeking robust evidence on how these approaches influence student engagement, learning behaviours, and academic outcomes.
Aim: This session explores how structured digital learning approaches and AI-enabled support can enhance student success in chemistry, and how these insights inform curriculum design choices such as continuous assessment, sequencing of content, and the integration of structured digital practice.
Materials and Methods: We analyse real-world data from undergraduate chemistry courses using structured, digitally mediated formative assessment, including weekly low-stakes testing and AI-supported study tools. Quantitative performance data is complemented by instructor observations and student feedback to provide a holistic view of learning impact.
Results: Across multiple cohorts, students engaging consistently with structured digital formative assessment demonstrate higher pass rates than those who do not. In first-year courses, overall pass rates were 55%, increasing to 63% among students successfully completing regular assignments and decreasing to 26% among those who did not. In second-year courses, overall pass rates were 79%, increasing to 87% for engaged students and decreasing to 55% for non-engaged students. While causality cannot be fully isolated—given that engaged students are often more motivated—the findings suggest that consistent, structured practice supports improved academic outcomes and sustained engagement.
Conclusion: Structured digital learning and AI-supported tools play an important role in supporting student progression in chemistry education. The findings highlight the value of embedding continuous formative assessment and structured practice as core curriculum design elements rather than optional enhancements. These insights support departments in making informed decisions about assessment strategies, student support mechanisms, and scalable digital integration.

WS - D1 - 1

Change and challenge in the chemical sciences: Universities, higher education and research across Europe

Universities across Europe are undergoing substantial change, affecting how chemical sciences education and research are delivered, funded and valued. This interactive workshop will explore how chemistry teaching, research, innovation and partnership models are evolving across European higher education systems. The session will involve hearing from speakers from across Europe each bringing complementary insights into current sector-wide shifts. Participants will also be invited to take part in breakout discussions to consider their own experiences, identify challenges and opportunities and share good practice. This session aims to bring a cross Europe chemical science dimension to understanding how universities are navigating and responding to rapid and significant change.

WS - D1 - 2
How can we make female pioneers in chemistry more visible, and why?

Lena Bonitz, Tomasz Pospieszny, Annette Lykknes, Brigitte van Tiggelen

Although we have achieved some success in gender equality, it is by no means guaranteed, and we must continue to defend it.
Mentoring programs are an important way to encourage girls and young women, in particular, to pursue careers in chemistry. However, looking to history is also a viable way to establish female role models, despite the different circumstances of the 19th and 20th centuries.
In the workshop, which will be moderated by Gisela Boeck, the chair of the History of Chemistry Division of the German Chemical Society (GDCh) at the University of Rostock, participants will discuss what young people hope to gain from researching and publishing the biographies of female chemists (statement by Lena Bonitz, the chair of the GDCh's Young Chemists' Forum, PhD-student at the Technical University Minors academy of Freiberg). Tomasz Pospieszny (professor in the Dept. of Bioactive Products at the Faculty of Chemistry at Adam Mickiewicz University in Poznań) will discuss his work related to Marie Skłodowska Curie's life and work in Poland. Annette Lykknes (Chair of the Division of the History of Chemistry at EuChemS and Professor in the Dept. of Teacher Education at the Norwegian University of Science and Technology in Trondheim) will discuss her motivation for focusing on women who contributed to the periodic table. Finally, Brigitte van Tiggelen, Director of International Affairs at the Science History Institute in Philadelphia, will present the Science History Institute's initiatives regarding women. During the concluding discussion, all participants will be invited to share activities in their respective countries. The discussion will explore ways to make all these successful projects more visible so their results can be utilized. One outcome of this workshop could be a collection of publications, books, films, and radio plays about female pioneers in chemistry that will be made available online later.

WS - D2 - 1
Responsible chemistry needs a global inclusive approach

Angela Agostiano (Chair), Pilar Goya, Nineta Hrastelj, Jan Mehlich, Ale Palermo, Sonsoles Martin Santamaria, Andrea Usenik
EuChemS Task Group 'Inclusion and diversity', European Chemical Society (EuChemS), BE

Can chemistry be truly responsible without embracing diverse global perspectives? The challenges we face - sustainability, safety, and resource use - are inherently global, and so are their consequences. This workshop explores why diversity of perspectives - gender-related, but not only - is not just about representation. It is about strengthening how we define problems, interpret uncertainty associated with risks, and anticipate impact. Join the conversation on how inclusive thinking, listening, and discussion can lead to better, more responsible chemistry.

Next European Research Programme: ‘Good chemistry’ between politics and science?

Márton Kottmayer
Science Europe, BE

The upcoming 2028-2024 Horizon Europe Programme[1] – following in the footsteps and sharing the name of its ongoing 2020-20727 iteration - is shaping up to be one of the biggest Research and Innovation Framework Programme of not only the European Union, but on the global scale as well[2].
Its stated goal is to support excellent research, breakthrough innovation, as well as collaborations that generate European added value – meaning that they can achieve more, than what national programmes would be able to so individually. Such cooperation within and beyond the EU is necessary to address global challenges through scientific means.
Yet, some of these global challenges are interlinked with the broader policy landscape, against the backdrop of which, Horizon Europe is being developed. This programme – and the research it will support – is being developed in a broader context, that is characterised by geopolitical paradigm shifts, that led the EU to an agenda prioritising autonomy and Competitiveness. This is why, in the current proposal, Horizon Europe is closely linked with a so called ‘European Competitiveness Fund’[3], an instrument that is expected to fund the EU’s strategic priorities. Yet, in this environment, it is crucial that science will not be subservient to these policy goals, rather it will complement them, maintaining key scientific principles and serving as a strategic priority in and of itself [4,5].
This workshop is being held at a critical point in time, just before the final inter-institutional negotiations on Horizon Europe are expected to begin. Thanks to this timing, it can reach beyond solely providing participants with a preliminary overview of the structure of EU level R&I funding. In addition, it can grant insights into the broader processes that drive these negotiations, the interconnectedness of expand on how the research community is involved.

[1]European Commission, COM/2025/544_1, **2025**
[2]CEPS, Towards an ambitious FP10, p1
[3]European Commission, COM/2025/555, **2025**
[4]Science Europe, Proposal for Amendments to the Council Decision & Regulation of the European Parliament and Council on establishing the 10th Framework Programme for Research and Innovation, **2026**
[5] Recommendations on Shaping the Close Connection Between Horizon Europe and the European Competitiveness Fund