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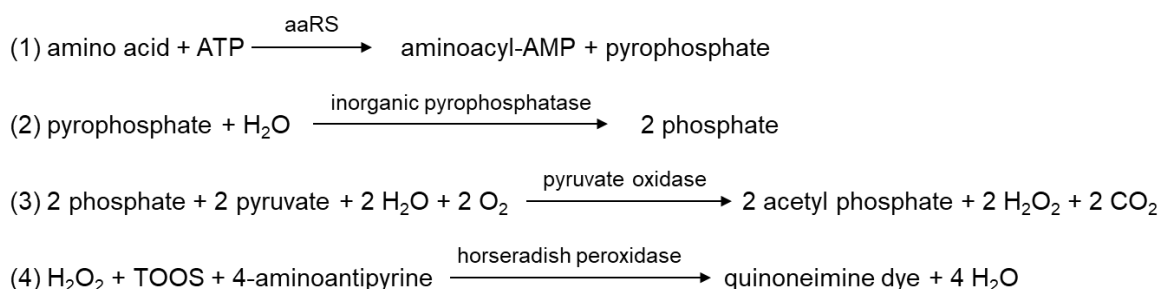
APC - D1 - P01

Development of paper-based analytical device for branched-chain amino acids

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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.

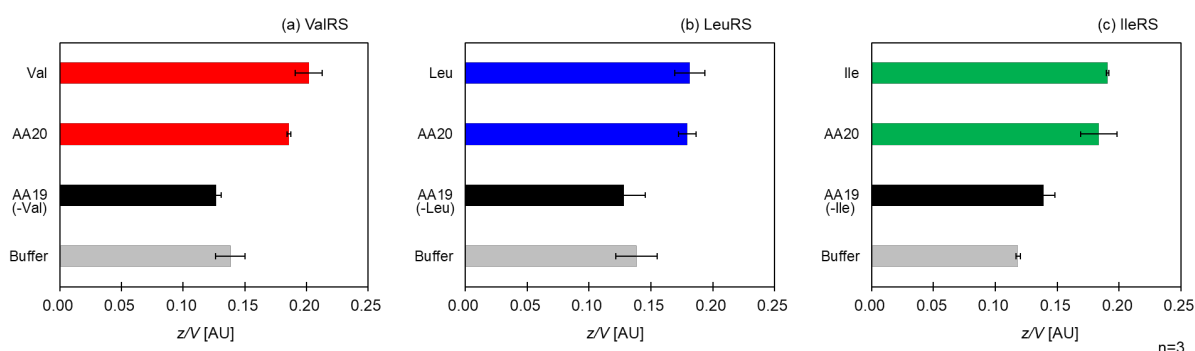


Fig. 1. Selectivity test for ValRS (a) using PADs. Substrate amino acid, 80 mM Val, a mixture containing 80 mM of 20 canonical amino acids (AA20), a 80 mM of 19 canonical amino acids excluding Val (AA19 (-Val)), and the reference buffer were applied to PADs. Similarly, (b) LeuRS and (c) IleRS.

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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 HNO₃ 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 (HNO₃-HCl-HF), which consistently yielded recoveries of approximately 100%. The '3 Acids + H₂O₂' 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 ₂ O 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%

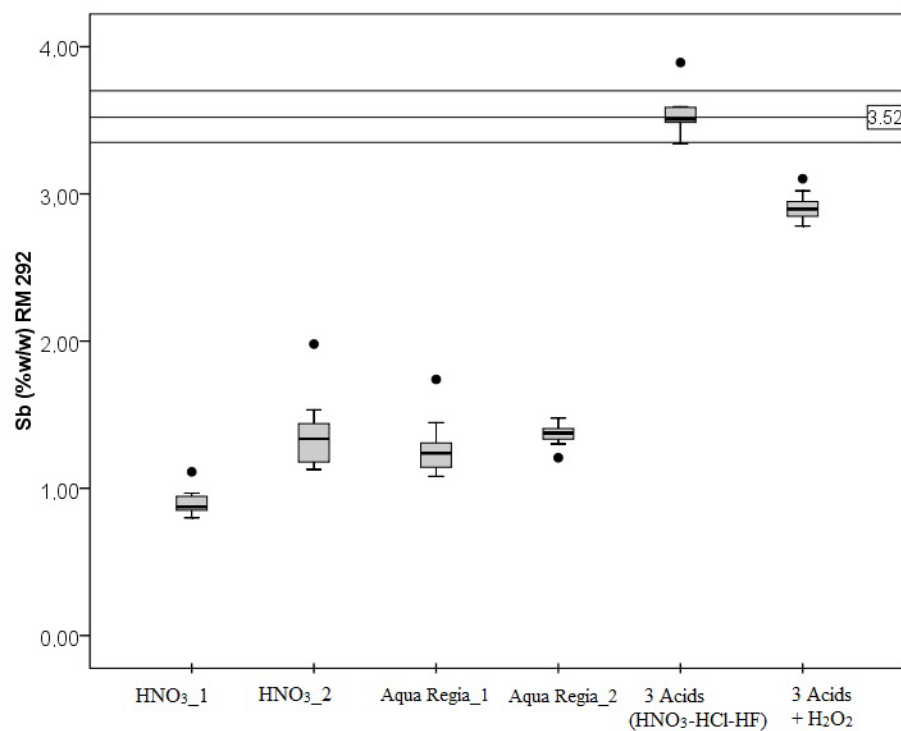
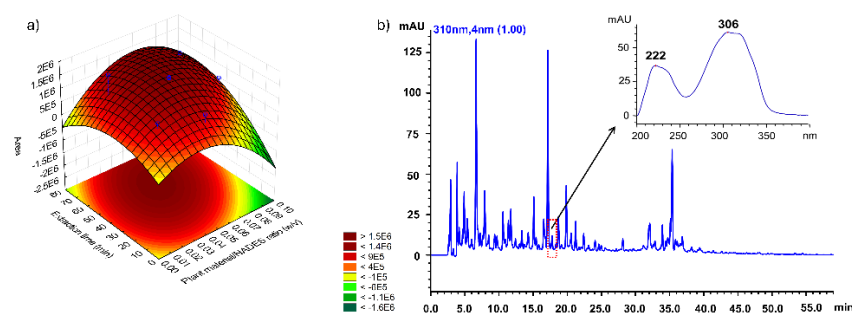


Figure 1. Antimony content (%w/w) boxplot from OREAS 292 Certified Reference Material using Different Dissolution Methods

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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 hypogaea* 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 (X₂), and 40 minutes of extraction (X₃).

Fig. 1. (a) Response surface of the significant variables (X₁ and X₃), 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 AGREE² (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.



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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 industry¹. 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 them². 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 performance³. 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.

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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 results¹. 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 cones⁵. 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 (CO₂), resulting in a homogeneous material containing the compounds of interest⁵. 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 hops².

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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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Assessment of the crystalline state of polymorphic pharmaceutical active ingredients in a forced degradation study utilizing seven recommended methodologies: Application to carbamazepine

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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 $40\pm 2^\circ\text{C}$ and $75\pm 5\%$ 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.

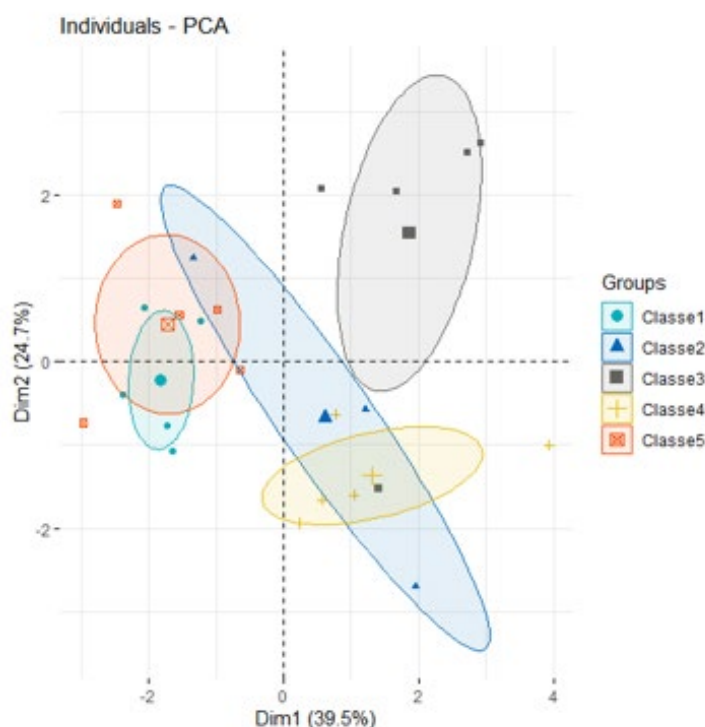


Fig. 1. illustrates the dispersion of crystalline properties across five batches, with classes 1, 2, 3, and 4 originating from the same manufacturer and class 5 sourced from a different manufacturer during the stability study.

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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.

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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 OpenChrom¹. 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 server³ (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)

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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)

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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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The 10th EuChemS Chemistry
Congress

12 - 16 July 2026

Antwerp, Belgium

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

Aditi Chandrasekar

Azim Premji University, India

Rapid industrialization intensifies environmental challenges by elevating atmospheric CO₂ levels, driving global warming, and ecosystem disruption. A promising approach to mitigate these adverse effects involves strategically utilizing anthropogenic CO₂ 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 CO₂ into epoxides predominantly rely on transition metal-based catalysts in conjunction with detrimental halide-containing co-catalysts. The current research¹ 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 CO₂ activation through carbamate intermediate formation.

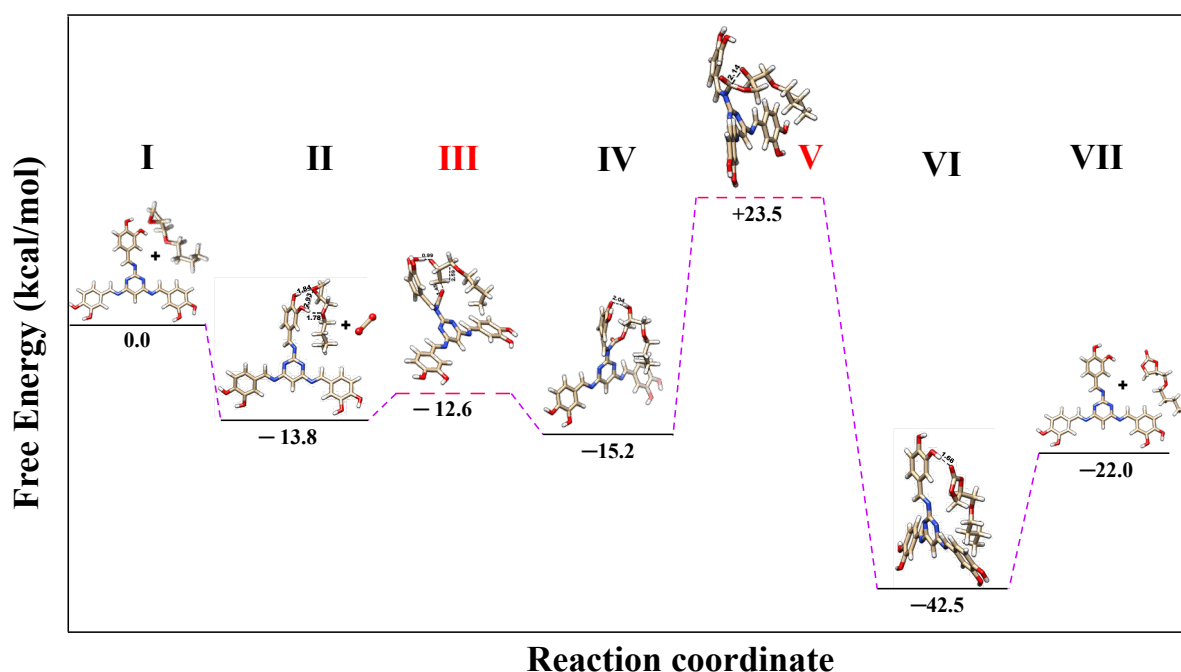


Fig. Reaction pathway along with the free energy associated with each step provided below the structure. The transition state structures are distinguished by dashed lines below them and minima geometries lie on solid lines. Interaction distances are provided in the inset.

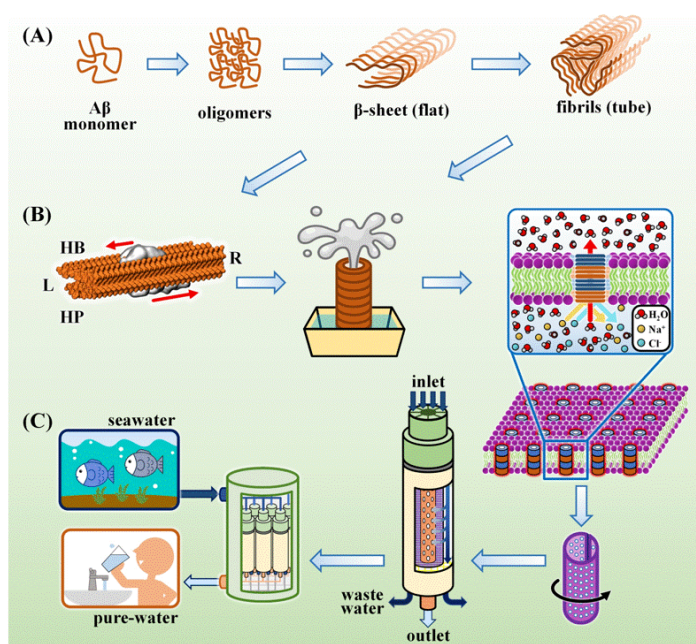
¹Hazarika, B.J., Paliwal, K.S., Mitra, A., Pan, P., Chandrasekar, A. and Mahalingam, V., *ChemCatChem*, **2025**, p.e01611.

Sheh-Yi Sheu¹¹Dept. 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 (A β) sheets owing to the ratchet structure of the underlying potential surface and the broken detailed balance. The water inside the self-assembled A β 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

¹Liu, Y. C.; Yang, D. Y.; Deng, J. P.; Sheu, S. Y.* *Small* **2023**, 2205420.

Lukas M. Sigmund¹¹AstraZeneca 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 Feurizer 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.

Predictive inorganic synthesis from small data using machine learning: Size-controlled Cu nanoparticles

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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]

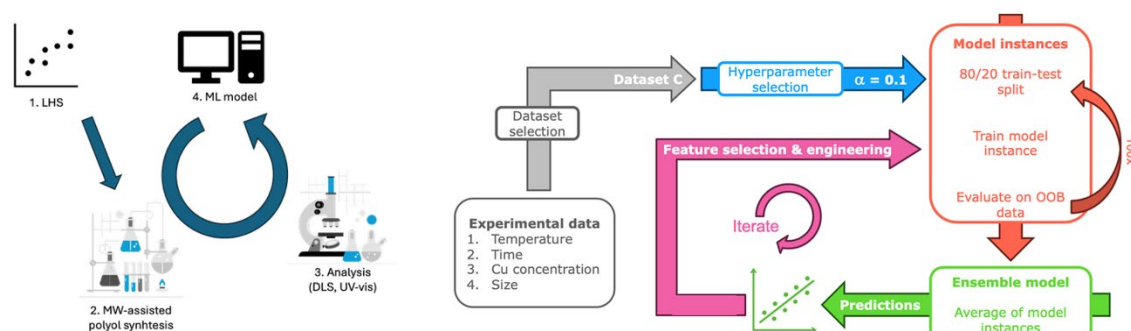


Fig. 1. Schematic representation of the synthesis workflow (left), with detailed workflow of the ML approach (right).^[3]

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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Defect mediated surface modification of amorphous TiO₂ surface using Grignard reagent in explicit solvation modelKrithika Ganesan¹, Erik C. Neyts^{1*}¹University of Antwerp, Belgium

Titanium dioxide is extensively employed in catalysis and energy conversion due to its inherent redox stability and adaptable surface chemistry¹. 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 anchoring², organometallic functionalization, particularly through the use of Grignard reagents, offers a direct pathway to form Ti–C bond formation³. 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 TiO₂ surfaces. A key focus was understanding how both intrinsic defects⁴ 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 TiO₂ surfaces using organometallic compounds.

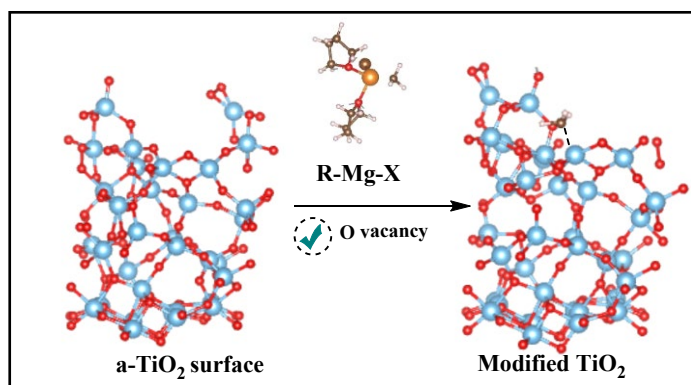


Fig. 1. Surface modification process of amorphous titania(a-TiO₂) using Grignard reagent(RMgX)

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 3 α -hydroxysteroid dehydrogenase and androsterone

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¹Kokushikan University, Japan; ²Health Sciences University of Hokkaido, Japan; ³Waseda University, Japan

Introduction: 3 α -hydroxysteroid dehydrogenase (3 α -HSD) is an oxidoreductase that catalyzes the following chemical reaction:



It is not still unclear how 3 α -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 3 α -HSD and how it is converted between oxidized and reduced forms. Therefore, we observed how 5 α -androsterone and 5 β -androsterone are incorporated into 3 α -HSD using molecular dynamics simulations.

1) As a structural model of 3 α -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, 5 α -androsterone (5 α -ANS) and 5 β -androsterone (5 β -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 (5 α -ANS or 5 β -ANS) was inserted into the 3 α -HSD model (2FVL (chain A) and NADP⁺) data. The initial position of androsterone was placed outside the 3 α -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 5 α -ANS or 5 β -ANS. We report on the structural changes of the entire 3 α -HSD molecule and the structural changes of NADP⁺ present in 3 α -HSD during the process of recognizing androsterone molecule. The results suggest that 3 α -HSD and NADP⁺ undergo considerable structural changes to accommodate the ligand molecule, depending on the shape of the ligand molecule.

Chemical accuracy in computational prediction of PFAS-cyclodextrin binding: A Multi-level sqm/qm study with experimental ITC validationChristopher J. Hobbs¹, Michal Řezanka¹, Stanisław Wacławek¹¹*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, historically, finding an adequate balance between computational cost and accuracy remaining 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), whereby 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 primarily 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 geometry¹. This validated workflow is robust and efficient, enabling computational screening of modified CDs and alternative PFAS structures for rational remediation system design.

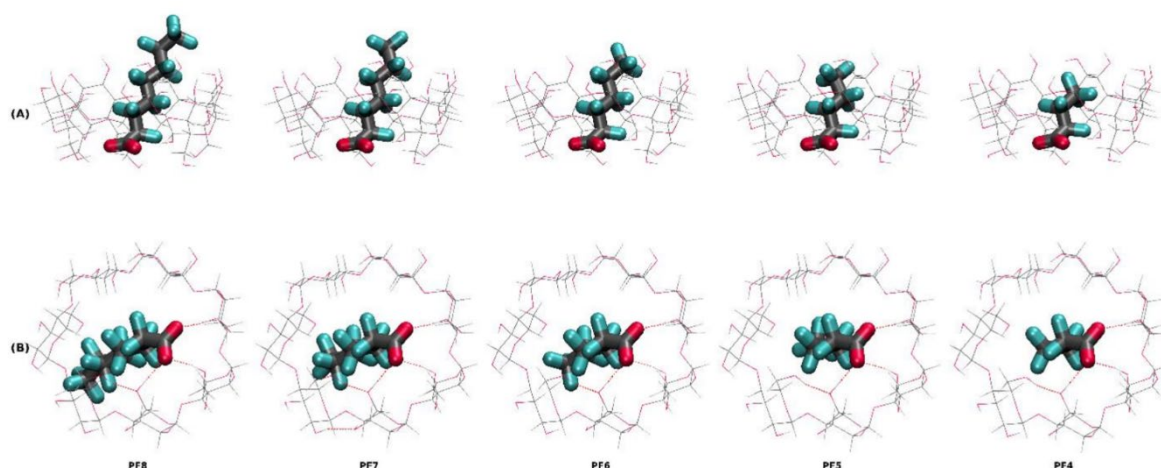


Fig. 1. Lowest-energy conformers of β -cyclodextrin complexes with perfluoroalkyl acids of varying chain length. (A) Side view; (B) top view from secondary rim, showing the H-bonding by red dashed line. PFAS: space-filling (cyan: CF₂/CF₃, red: COO⁻); cyclodextrin: line representation.

¹Jameel, F.; Stein, M. *Phys. Chem. Chem. Phys.* **2024**, 26, 21197–21203.



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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*

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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.

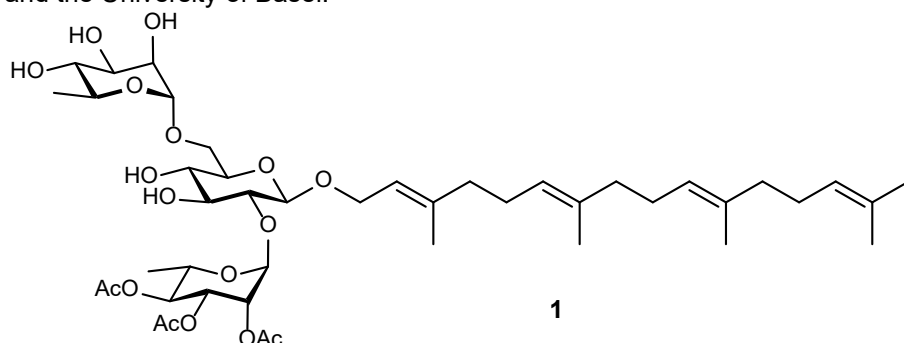


Fig. 1. Structure of plant-derived glycoside **1**

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Peptide conformation engineering on a chitosan nanowhisker–graphene oxide interface enables high-performance electrochemical detection of food allergen

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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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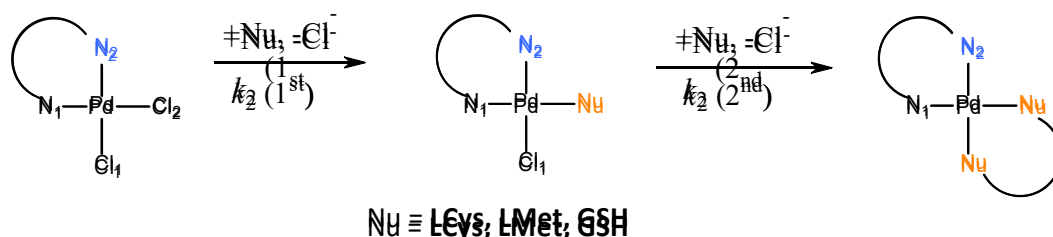
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Tuning the reactivity of *N,N'*-Pyridyl palladium(II) complexes: A substitution kinetics and DNA/BSA binding study

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¹University 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 ¹H-NMR, ¹³C-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.

¹Ferraro, M.G; Piccolo, M; Misso, G; Santamaria, R; Irace, C. *Pharmaceutics*, **2022**, 14, 954.

²Bugarčić, Ž.D; Bogojeski, J; van Eldik, R. *Coordination Chemistry Reviews*, **2015**, 292, 91-106.

Synergistic cancer therapy targeting LAG-3&PD-L1 through co-administration of flavonoid and durvalumabKonrad Barnowski^{1,2}, Wen Zhang³, Judyta Cielecka-Piontek⁴, Łukasz Skalniak¹, Jacek Plewka¹¹Faculty of Chemistry, Jagiellonian University, Poland; ²Doctoral School of Exact and Natural Sciences, Jagiellonian University, Poland; ³College of Pharmaceutical Science, Zhejiang University of Technology, China; ⁴Faculty 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 phase¹.

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, $K_D=4.6\ \mu\text{M}$) and its blockade of LAG-3/MHCII interactions (HTRF, $\text{IC}_{50}=19.3\ \mu\text{M}$), 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).

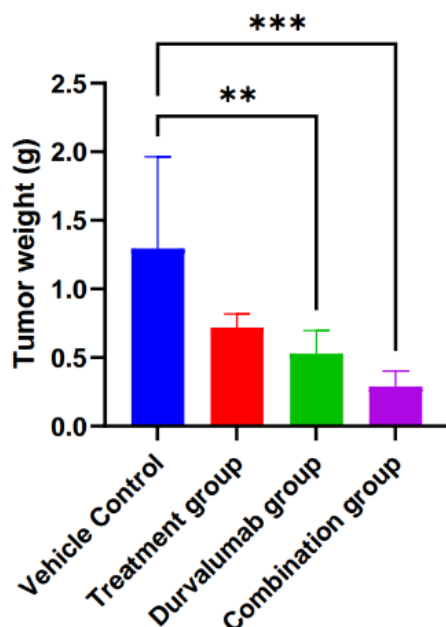


Fig. 1. Synergistic anticancer effect of co-administration of flavonoid and anti-PD-L1 antibody durvalumab on reducing murine tumor weight.

¹Abdel-Rahman, S. et al. *ACS Med. Chem. Lett.* **2023**, 14(5), 629-635.

Denys Bondar¹, Steven P. Nolan¹¹UGent, 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 ⁷⁷Se NMR chemical shifts correlate with Tolman electronic parameters (TEP), revealing the relationship between donor strength and metal–ligand dynamics.

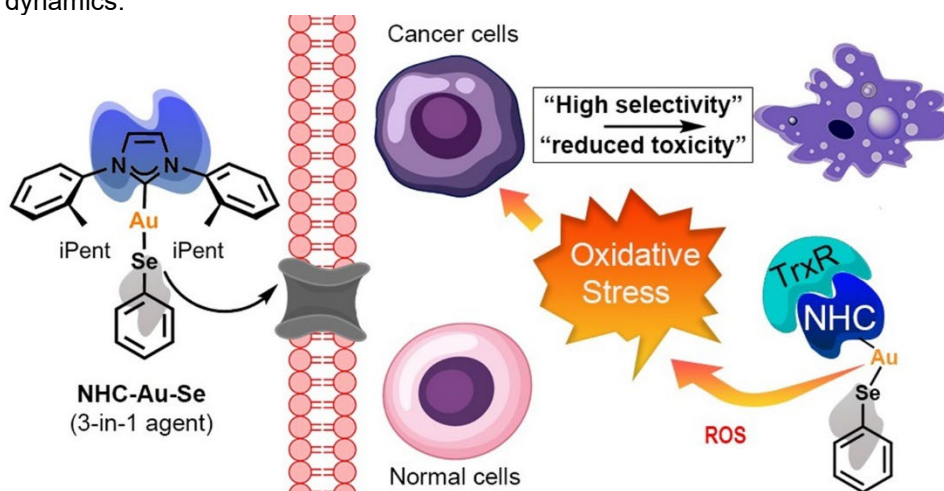


Fig. 2. Concept of the DoNoHarm project.

The lead compound, Au(MonoIPent)SePh (1m), displays sub-micromolar cytotoxicity ($IC_{50} \approx 0.3 \mu M$) 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).

¹Arnaut, P.; Bracho Pozsoni, N.; Bondar, D.; et al. *Chem. Sci.* **2025**, *16*, 17221–17231.

²Ott, I.; Nolan, S. P. *Chem. Rev.* **2023**, *123*, 10211–10268.

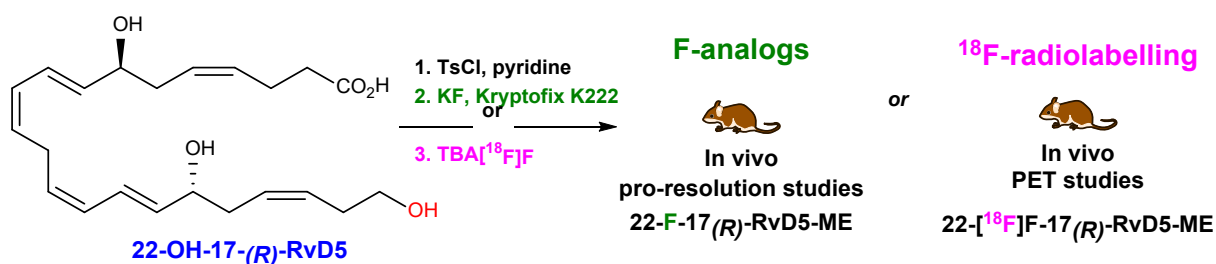
³Tzouras, N. V.; Scattolin, T.; Cavarzerani, E.; Nolan, S. P. *Chem. Rev.* **2021**, *121*, 6888–6954.

CBF - D1 - P06

Stereoselective synthesis of ^{18}F -labelled specialized pro-resolving mediators

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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 synthesized, including the ^{18}F -labeled analog that is shown in the scheme below. The radiolabeled compound may be used for positron emission tomography (PET) studies², which could provide new insights into how the analogs are distributed *in vivo*, as well as their pharmacokinetics, and target tissue engagement.



¹Luo, X.; Gu, Y.; Tao, X.; Serhan, C.N.; Ji, R.R, *Front. Pharmacol.* **2019**, *10*,

²Tungen, J. E.; Aursnes, M.; Ramon, S.; Colas, R. A.; Serhan, C. N.; Olberg, D. E.; Nuruddin, S.; Willoch, F.; Hansen, T. V. *Org. Biomol. Chem.* **2018**, *16*, 6818.

CBF-D1 - P07

Optimization of SPME–GC-MS for volatile profiling and botanical origin discrimination of Portuguese monofloral honey

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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

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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).

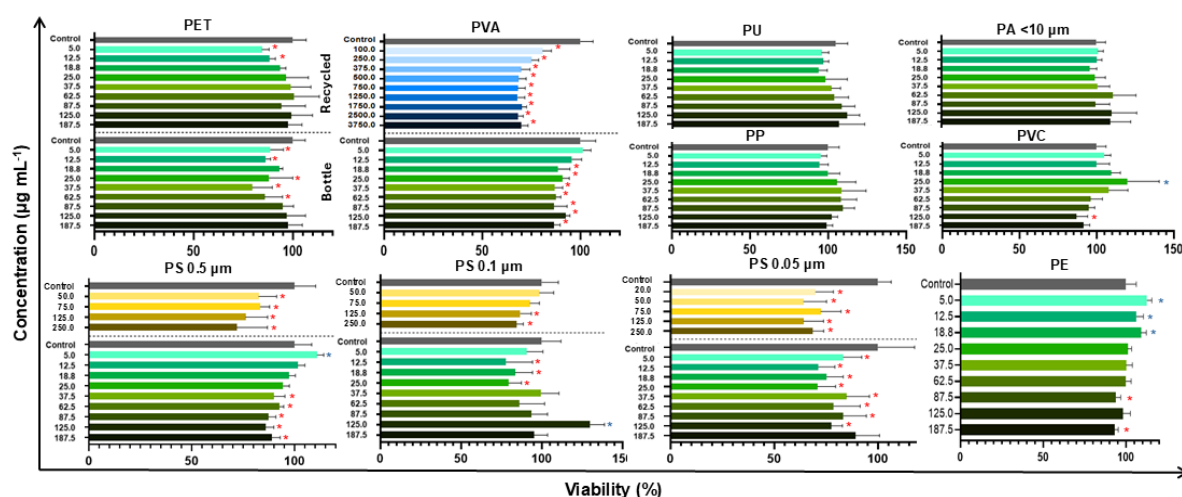


Fig. 1. Cell viability graphs for analyzed plastic particles. Concentrations with statistically lower viability than the control ($p < 0.05$) are marked (*), and those with statistically higher viability ($p < 0.05$) are marked (*)

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).

¹Zhang et al.; *Earth Sci Rev* 2020, 103118.

CBF - D1 - P09

Development and validation of analytical performance of ICP-MS blood lead testing method using the ICHM10 new protocol for bioanalytical method

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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 45 µg/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® 350X 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 (01 µg/L) to ULOQ (1500 µg/L) included blank and zero samples. Calibration and quality control (QC) solutions at three levels, low at 1.5 µg/L, medium at 75.0 µg/L, and high at 900.0 µg/L, were prepared by overloading whole blood from a standard solution of 1,000 ± 0.002 g/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%).

¹Institute for Health Metrics and Evaluation. GBD Compare. <http://vizhub.healthdata.org/gbd-compare>

²Organization WH. The public health impact of chemicals: knowns and unknowns: data addendum for 2019. 2021. <https://iris.who.int/handle/10665/342273>

³Lignes Directrices de l'OMS Sur la Prise en Charge Clinique de l'exposition Au Plomb: Résumé Analytique. 1st ed. Geneva: World Health Organization; 2021. 1 p.

⁴ICH M10 sur la validation des méthodes bioanalytiques - Guide scientifique | Agence européenne des médicaments (EMA). <https://www.ema.europa.eu/en/ich-m10-bioanalytical-method-validation-scientific-guideline>

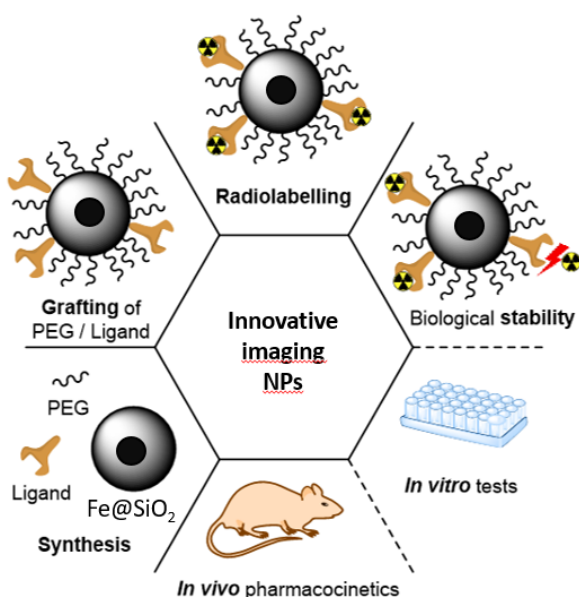
CBF - D1 - P10

Innovative radiolabelled magnetic nanoparticles for dual MRI/SPECT imaging

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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 careful 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.



¹Mathieu, P.; Coppel, Y.; Respaud, M.; Nguyen, Q. T.; Boutry, S.; Laurent, S.; Stanicki, D.; Henoumont, C.; Novio, F.; Lorenzo, J.; Montpeyo, D.; Amiens, C. Silica Coated Iron/Iron Oxide Nanoparticles as a Nano-Platform for T2 Weighted Magnetic Resonance Imaging. *Molecules* **2019**, *24* (24), 4629.

CBF - D1 - P11

High-throughput serum metabolomics for PFAS toxicity- method development and cohort validation in Belgian residents near a PFAS production plant

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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.

Green extraction of pomegranate peel unlocks ellagitannin-driven longevity pathways

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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/H₂O 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.

¹Altieri, F. et al., *Nutr.* **2019**, 11(1), 186.

²Balli, D. et al., *Antiox.* **2020**, 9(3), 238.

³Martel, J. et al., *Micr. Cell.* **2020**, 7(10), 255.

CBF - D1 - P13

Pesticide residues in commercial honey samples: Application of a validated analytical method and chemometric interpretation

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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.



The 10th EuChemS Chemistry
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Catalyzing New Chemistry Solutions (CCS)

Lisa De Vriendt¹, Ibrahim Khalil², Matthew Hickson¹, Bert Sels¹, Michiel Dusselier¹¹KU Leuven (CSCE), Belgium; ²Lyon 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 RuCl₃·3H₂O 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.

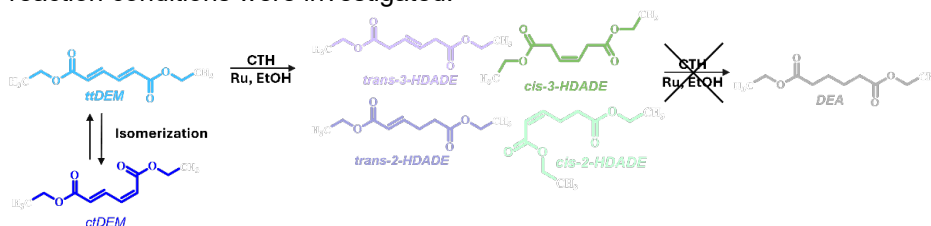


Fig. 1. Overview of the CTH of *cis*,*trans* and *trans*,*trans*-diethyl muconates (*ct*DEM and *tt*DEM) towards HDADE (hexenedioic acid diethyl ester, 4 isomers), with the goal to avoid the full hydrogenation towards diethyl adipate (DEA).

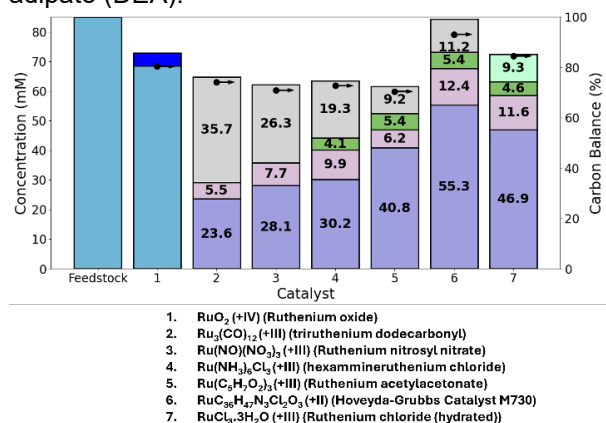


Fig. 2. Results of the catalytic screening of different Ru precursors (RuO₂, Ru₃(CO)₁₂, Ru(NO)(NO₃)₃, Ru(NH₃)₆Cl₃, Ru(C₅H₇O₂)₃, RuC₃₆H₄₇N₃Cl₂O₃ and RuCl₃·3H₂O) in the transfer hydrogenation of *tt*DEM (diethyl muconate). Reaction conditions: 85 mM *tt*DEM, 5 mL EtOH, 175 °C, Ru/MA (mol/mol) = 1/50, 14 bar N₂, 5 hours. Colors correspond to figure 1.

¹Khalil, I. Quintens, G. *Green Chemistry* **2020**, 22 (5), 1517–1541.

²Khalil, I. Rammal, F. *Green Chemistry* **2024**, 26, 5852–5861.

³Khalil, I. Rigamonti, M. *Nat Catal* **2024**, 7 (8), 921–933.

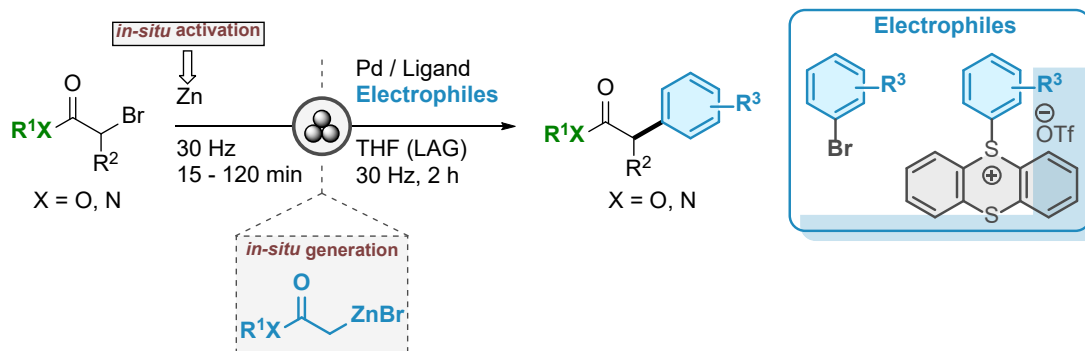
⁴Carter, P. Meyer, P. M. *RSC Sustainability* **2024**, 2, 2968–2978.

⁵Dell'Anna, M.N. Laureano, M. *Green Chemistry* **2021**, 23 (17), 6456–6468.

⁶De Vriendt, L. Khalil, I. *ChemCatChem* **2025**, 17 (19).

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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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Synergistic graphene/CuO coatings by an intermittent spray-coating to enhance the thermal decomposition and performance of ammonium perchlorate

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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 performance¹.

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 particles².

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 reduction³. 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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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 conversion¹.

Perovskites (LaMnO₃, LaCoO₃, LaNiO₃) 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: LaMnO₃ favored branched olefins (3-methyl-1-butene and 2-methyl-1-butene), LaCoO₃ favored aldehydes (2-methylpropanal), and LaNiO₃ produced ketones such as 4-methylpentan-2-one. Raising temperature to 600°C shifted LaMnO₃/LaCoO₃ toward light carbonyls (acetaldehyde as dominant, with propanal and butanal), whereas LaNiO₃ 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 C₂–C₅ carbonyls, C₄ 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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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 strength¹ (Figure 1). However, the recent emergence of dynamic catalysis offers a promising route to overcome these constraints¹. 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 limit¹. 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 CO₂ to methanol and methanation. In this work, a benchmark static catalyst system was first developed using commercial catalysts (Ni/SiO₂, Cu/ZnO/Al₂O₃) 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.

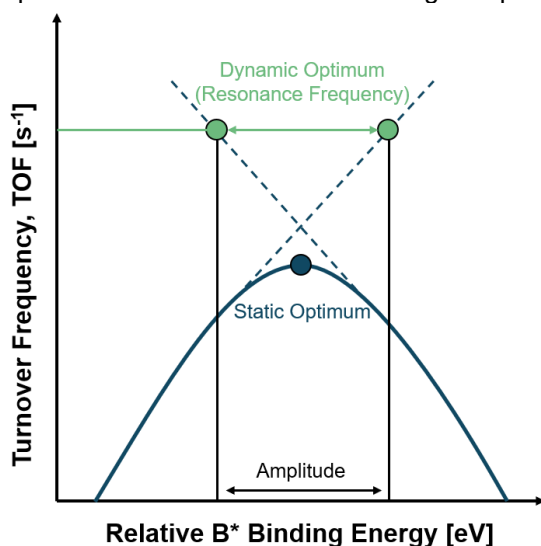


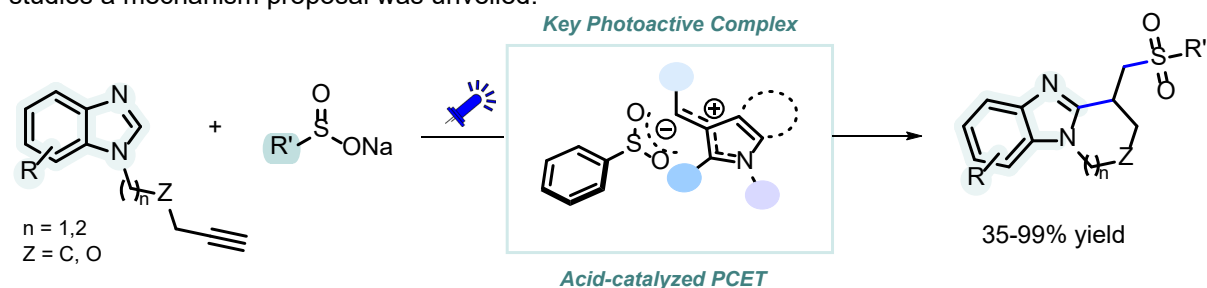
Fig. 1. A representation of dynamic catalysis. The optimum of a static catalyst highlighted at the apex of the Sabatier volcano plot, whereas a higher catalytic rate for a dynamic catalyst can be found at a maximum known as the resonance frequency. Adapted from [1].

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Radical cascade sulfonylation/cyclization of benzenimidazole derivatives with sulfinates induced by visible lightPolyssena Renzi¹, Davide Cerrina¹, Giovanni Ghigo¹, Annamaria Deagostino¹¹Dept. of Chemistry, University of Turin, Italy

Organosulfur moieties are key features in numerous natural products¹ 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 diarylmethyl cation 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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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 H₂ 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.

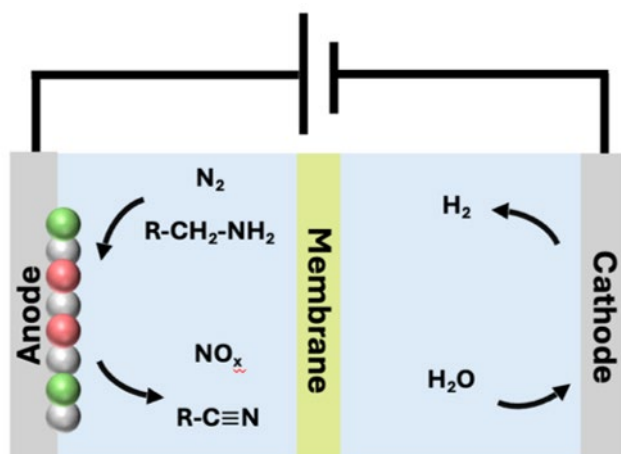


Fig.1. Electrocatalytic oxidation of nitrogen compounds on immobilized metal oxide materials

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The catalytic hydrogenation of CO₂ 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°C. Limiting the calcination temperature to 330°C favors the formation of smaller Cu⁰ 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} H₂ 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 H₂/CO₂ = 3 demonstrate that the CuZnGa catalyst calcined at 330°C exhibited significantly higher CO₂ 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 CO₂-to-methanol conversion.

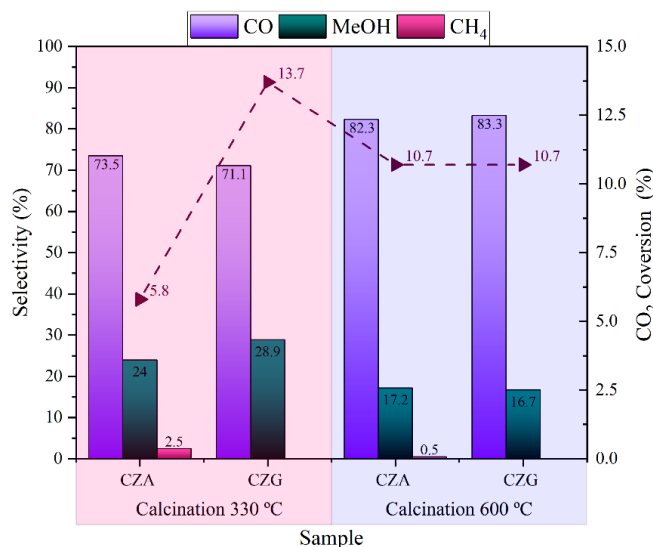


Fig. 1. Catalytic tests of the materials calcined at 330 °C or 600 °C

The authors acknowledge the financial support from FAPESP – São Paulo Research Foundation (Process N°. 2024/00032-4 and Process N°. 2025/09667-5) and from CNPq (Process N° 300454/2025-2).

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Turpentine oil, a byproduct of the paper industry, is a very attractive and highly available raw material. The main constituent of turpentine is α -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 α -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 α -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 α -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 α -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.

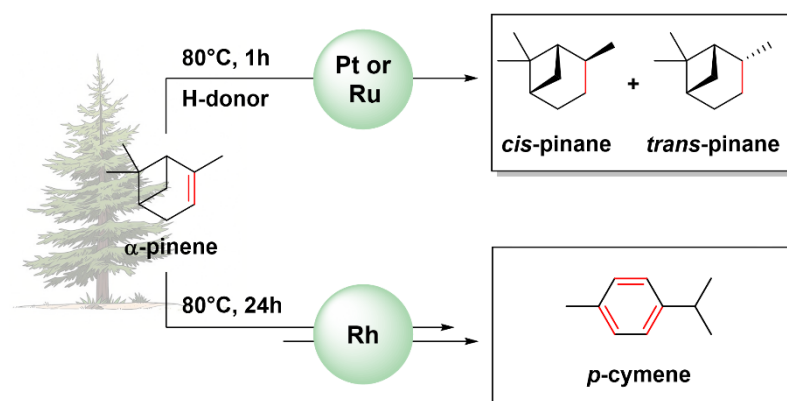


Fig. 1. Conversion of α -pinene to pinane and to *p*-cymene.

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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

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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 gaseous⁴ 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.

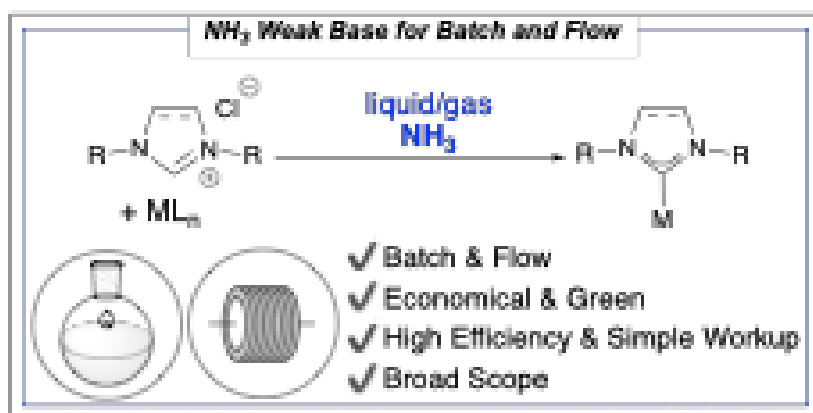


Fig. 1. Ammonia-mediated synthesis of metal-NHC complexes in batch and flow approaches.

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Digold photosensitizer for visible light [2+2] cycloaddition and E/Z isomerization reactions

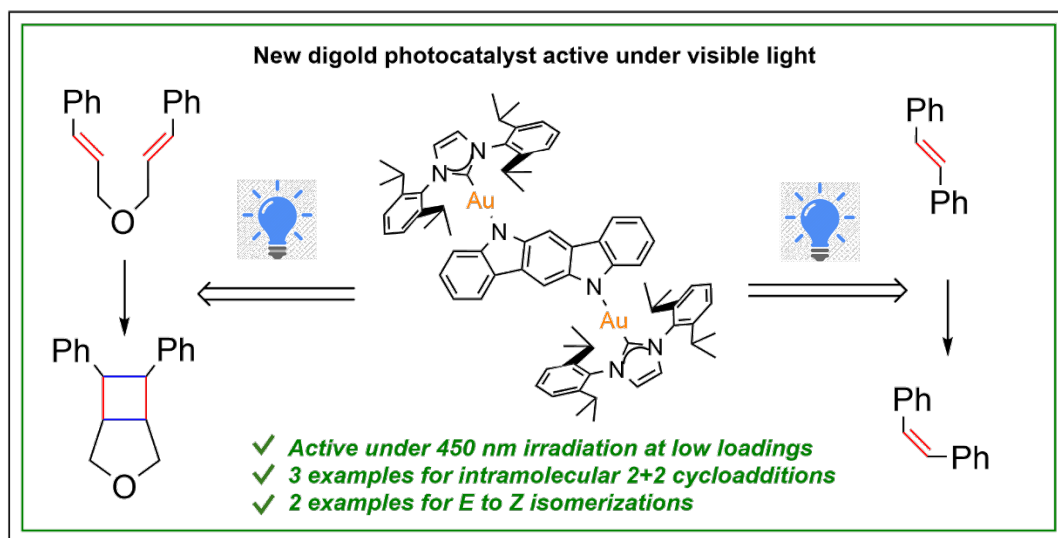
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Energy transfer photocatalysis has emerged as a powerful platform for a wide variety of transformations, yet advances in this area are often limited by the visible-light absorption of catalysts and the very high cost of state-of-the-art iridium-based 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 μ s. 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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Growing scientific and technological interest in the valorization of carbon dioxide has intensified research on CO₂ hydrogenation to methanol (CO₂-MeOH). This reaction is attractive as a route for CO₂ mitigation, as a power-to-liquid energy storage option, and as an alternative pathway to conventional syngas-based methanol synthesis. Nevertheless, CO₂-MeOH remains highly challenging because of unfavorable thermodynamics, the chemical stability of CO₂, the occurrence of parallel reactions, and catalyst deactivation.

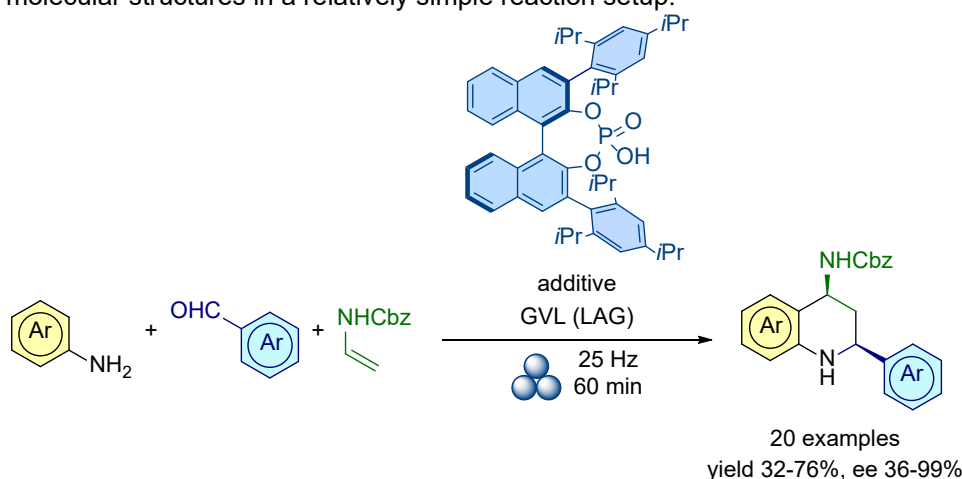
In this work, MOF-derived carbon was employed as a modifier for Cu/ZnO/Al₂O₃ (CZA) catalysts with a Cu:Zn:Al molar ratio of 6:3:1. The aim was to simultaneously increase the specific surface area, improve copper dispersion, and enhance water resistance of the catalysts, due to the hydrophobic character 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 Na₂CO₃ 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 CO₂ and H₂ adsorption properties, indicating promising potential for improved catalytic performance in CO₂ 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 H₂/CO₂ = 3–6 molar ratios.

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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 stereinduction 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

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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 industry³. 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.

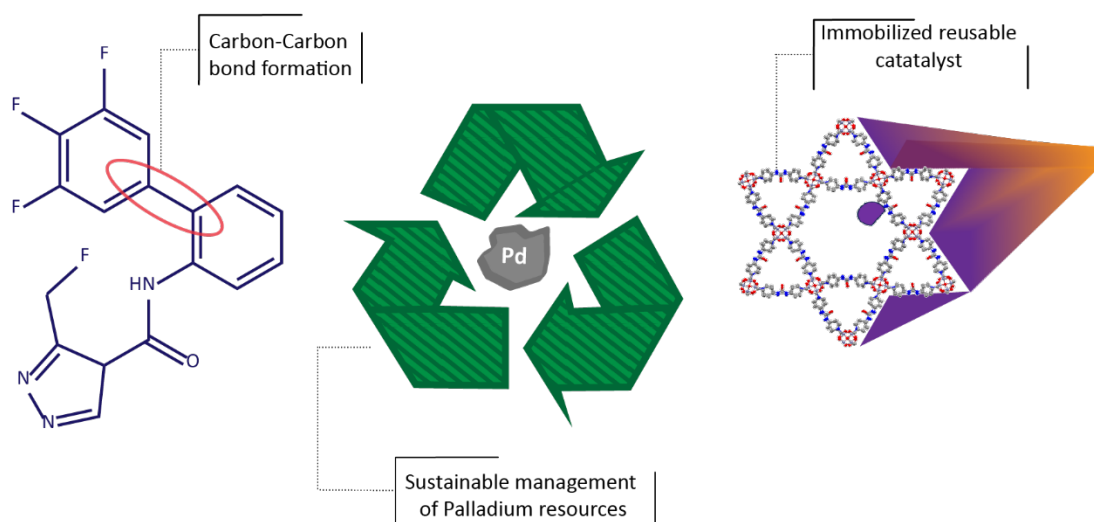


Fig. 3. visual abstract of Immobilized pincer ligand for cross-coupling reaction in flow

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Potential of tubular continuous flow photoreactors for plasmonic photocatalytic reverse water gas shift process

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CO₂ 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 CO₂ and green H₂ are converted into CO and H₂O. The resulting CO, together with H₂, 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 CO₂.²

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 m² 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 m² of illuminated catalyst bed, while also identifying the limitations of the setup. Using a TiO₂-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·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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In this modern and industrial society, it is vital to find solutions for converting CO₂ 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 CO₂ conversion processes.

Although both alumina and silica supported metal catalysts are valued for their improved properties, like strong metal-support interactions, acid-base sites, CO₂ 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 CO₂ 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 CO₂ 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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Due to the growing interest in CO₂ valorization pathways, CO₂ hydrogenation to methanol (CO₂–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 CO₂–MeOH are the competitive reverse water gas shift reaction (RWGS), which leads to low methanol selectivity at higher CO₂ conversion, as well as catalyst deactivation due to water formation. In this regard, one strategy in designing selective and stable catalysts for CO₂–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-Al₂O₃ (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 group¹. 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 Na₂CO₃ or NaHCO₃ 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, H₂/CO₂-TPD, FT-IR, DRIFTS, and N₂O titration revealed uniform dispersion of the components, enhanced surface area due to carbon modification, better reducibility, and different interactions with H₂ and CO₂, with subsequent differences in catalytic performance in the CO₂–MeOH process.

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Phthalocyanines (Pcs) are macrocyclic molecules that exhibit high aromatic character due to their conjugated 18 π -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.

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Unravelling surface mechanism in isopropanol dehydration to propylene: The impact of acid-base sites strength and nature

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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.

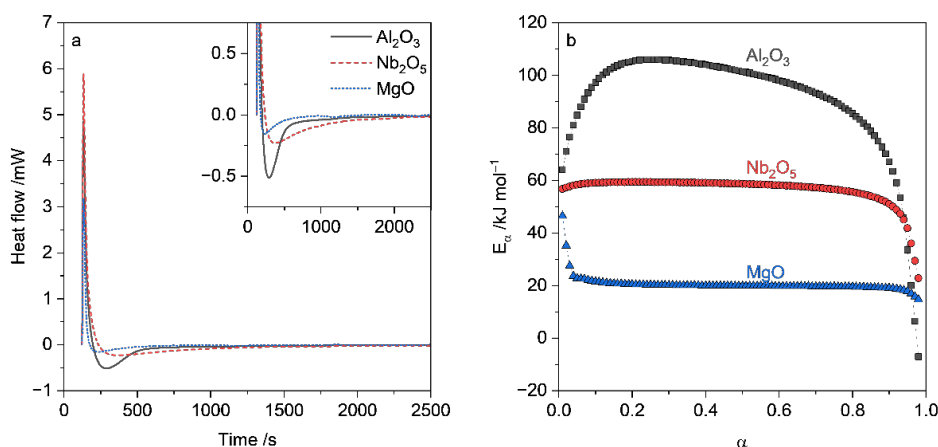


Fig. 4. Calorimetric signals recorded after IPA pulses (a) and related dependences of the effective activation energy versus the extent of conversion (b) obtained on alumina (solid, black), niobium oxide (dash, red) and magnesium oxide (dot, blue) at 175 °C.

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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Nanostructured molybdenum sulphide encapsulated in carbon spheres as stable and efficient electrocatalysts for the hydrogen evolution reactionRebeca Molina-Bueno¹, David Ruíz-Almóguera¹, José A. Mata¹, Iván Sorribes¹¹*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 $-10 \text{ mA}\cdot\text{cm}^{-2}$ 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.

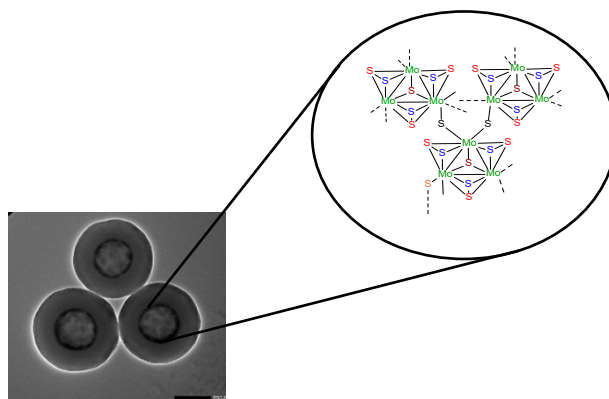


Fig. 1. Nanostructured molybdenum sulphide encapsulated into carbon spheres

Acknowledgements: 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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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 (MoS₂)-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 MoS₂-type nanomaterials. The resulting {Mo₃S₄₋₇}_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 (TiO₂), a widely used UV-responsive photocatalyst, result in efficient photocatalysts towards the hydrogen evolution reaction (HER) from water. Furthermore, {Mo₃S₇}_n has been shown to function as a universal co-catalyst, exhibiting effective activity when combined with other inorganic semiconductors (g-C₃N₄, CdS, and MXene) as well as organic photosensitizers (erythrosine B sodium salt and eosin Y).

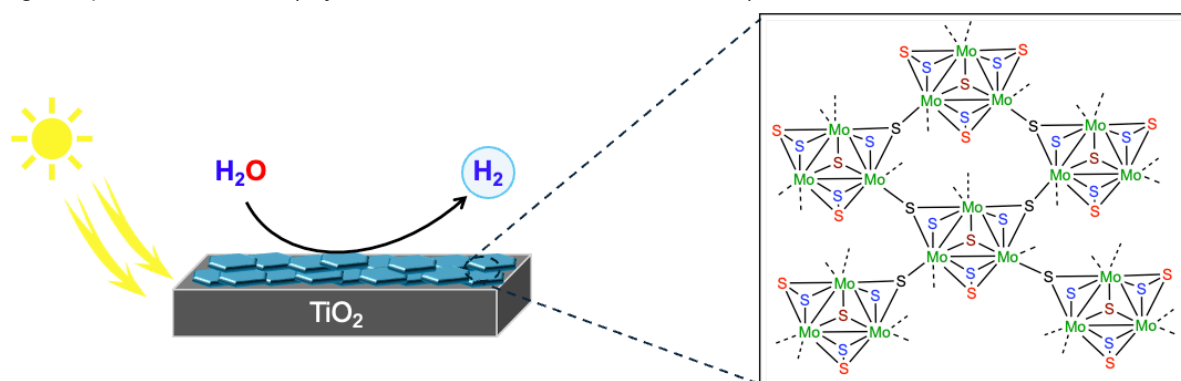


Fig.1. Photocatalytic HER catalysed by {Mo₃S₄₋₇}_n/TiO₂ nanocomposites

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 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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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 $\{\text{Mo}_3\text{S}_4\}_n$, 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.

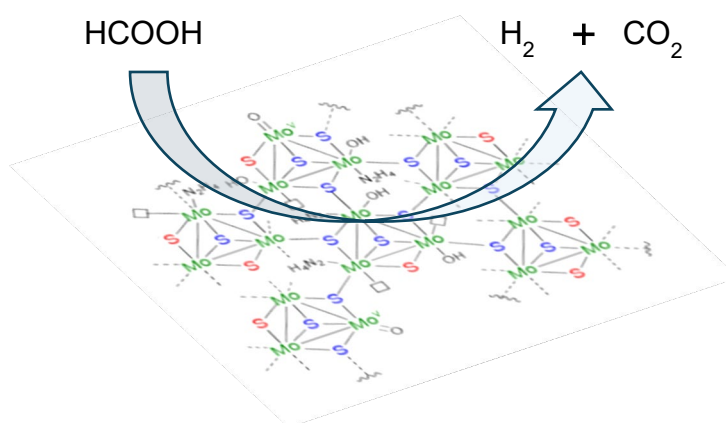


Fig. 5. $\{\text{Mo}_3\text{S}_4\}_n$ -catalysed dehydrogenation of formic acid

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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The concern over rising CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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/SiAlO_x and Ni_xCo_y/TiO₂), and their performance in the RWGS. Our results show that the Ni:Co ratio results in changes in the electronic and structural properties that lead to different selectivity and activity.

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Alkali-promoted iron-based catalysts for efficient and selective CO₂ hydrogenation to light olefin: A combined mechanistic and DFT insightsBabar Ali¹, 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 CO₂ to light olefins over alkali-promoted iron catalysts offers a sustainable pathway for CO₂ utilization and production of valuable chemicals. This study investigates the effect of alkali (Na, K, Cs) promotion on Fe-based catalysts for CO₂ hydrogenation to light olefins. Characterization techniques revealed that alkali promoters enhanced CO₂ adsorption, activation, and catalyst basicity, while weakening H₂ binding and facilitating desorption, shifting selectivity toward light olefins (C₂-C₄). The K-promoted catalyst achieved 38.3% olefin selectivity at 44.7% CO₂ conversion, attributed to stabilization of χ -Fe₅C₂ and suppression of alkene hydrogenation via moderate electron donation. In contrast, Na delayed Fe reduction and promoted heavier hydrocarbons, while Cs showed weak CO₂ uptake. XPS analysis revealed that K promotion enhances iron carburization, stabilizing the active χ -Fe₅C₂ phase and increasing the C-Fe fraction, which favors light olefin formation. In contrast, Na promotion leads to more oxidized Fe²⁺/Fe³⁺ 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 CO₂ 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 CO₂ adsorption behavior of Fe₂O₃ surfaces, with the (110) facet being the most active. K doping provided optimal adsorption energy (-0.80 eV) and balanced charge transfer, enhancing CO₂ activation and light olefin selectivity. In contrast, Na led to over-strong adsorption, resulting in heavier hydrocarbons, while Cs showed weak CO₂ binding and low activity.

Keywords: CO₂ hydrogenation, Iron Catalyst, olefins, alkali promoters, Iron carbide

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Energy, Environment & Sustainability (EES)

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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 data⁷ 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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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 IrO₂ 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.

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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 $\lambda_{\text{excitation}} = 230$ nm. Studies involving 12 interferents showed that nanolignin had high selectivity for Cr(VI) fluorometric detection, with $\lambda_{\text{excitation}} = 340$ 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 $\mu\text{mol L}^{-1}$, 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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Dimethyl Ether (DME, CH₃OCH₃) 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 CO₂ with renewable H₂ 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.

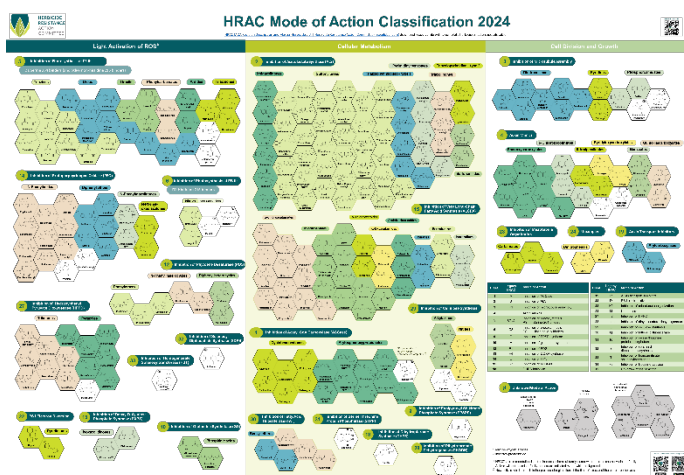
By integrating renewable carbon sources with such advanced utilization technologies, DME acts as a crucial bridge linking sustainable production to multi-sectoral decarbonization, reinforcing its pivotal role in building a resilient and carbon-neutral energy future.

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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 members⁸ have been taken up.

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Hydrophilic bipyridine–sulfonate polymeric colloids as stable redox electrolytes for aqueous organic flow batteries

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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, ¹H/¹³C 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.

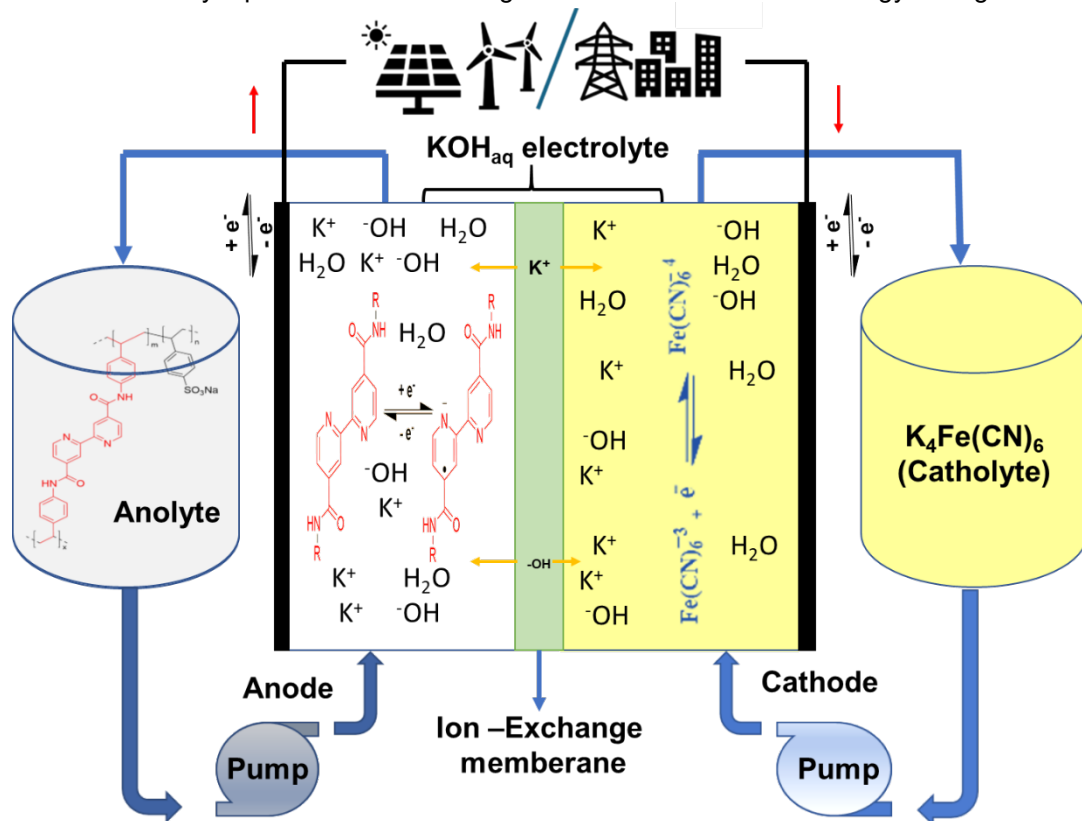


Fig. 1. Graphical Abstract

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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 ($S_{\text{load}} > 3 \text{ mg cm}^{-2}$) and restricted electrolyte amounts ($E/S < 8 \text{ } \mu\text{L mg}^{-1}$)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 cathodes². These challenges critically hinder sulfur electrokinetics under lean electrolyte conditions³. 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 interface¹. 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 $\mu\text{L mg}^{-1}$ 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.

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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.

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The growing demand for efficient and sustainable water treatment technologies has intensified interest in converting industrial solid waste into value-added functional materials¹. 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 capture².

Adsorption experiments were carried out using representative organic pollutants commonly found in contaminated effluents². 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 involved².

The results demonstrate that converting industrial waste into functionalized adsorbents offers a promising, low-cost and environmentally responsible alternative for sustainable water treatment³. 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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The efficient valorisation of CO₂ into higher value products is a key strategy for mitigating greenhouse gas emissions and enabling sustainable chemical production. Direct CO₂ hydrogenation to ethanol is particularly attractive, yet it remains challenging due to limited selectivity and productivity of most catalytic systems¹. Here, we demonstrate a highly active and stable series of alkali-promoted trimetallic catalysts for gas-phase CO₂ 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·g_{cat}^{−1}·h^{−1} ethanol STY at 300 °C and 20 bar, with H₂/CO₂ = 3 and GHSV = 9917 h^{−1}, representing one of the highest reported space-time yields among non-noble metal catalysts². The corresponding CO₂ conversion reached 17%, while C₂⁺ 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 CO₂ activation and C–C coupling. Catalyst structure and surface chemistry were analysed using XRD, BET, SEM/STEM-EDX, XPS, CO₂-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 CO₂ adsorption, but hindered ethanol selectivity due to stronger binding and side reactions. This study demonstrates that precise alkali promotion of trimetallic catalysts enables efficient CO₂-to-ethanol conversion, providing new insight into catalyst design for scalable, sustainable fuel and chemical synthesis.

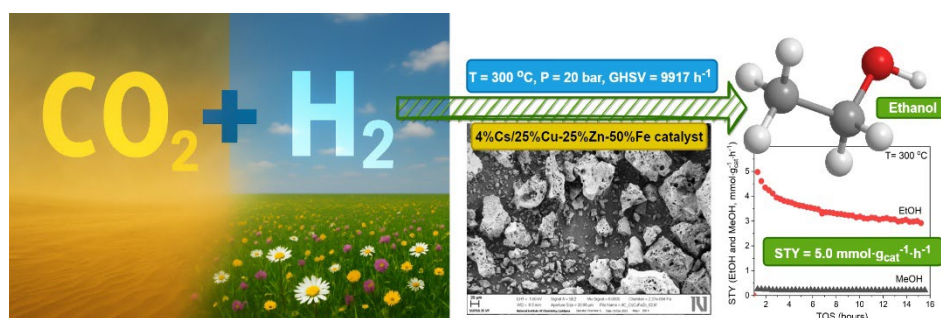


Fig.1. Schematic representation of CO₂ hydrogenation to ethanol over a high-performance catalyst.

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Development of plant growth-promoting bacteria with artificial humic acids capsules for enhanced agricultural sustainability

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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.

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The continuous rise in atmospheric carbon dioxide (CO₂) 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 CO₂ 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 CO₂ 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 CO₂ 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.

Synthesis of nickel-based catalysts for the (photo)thermocatalytic production of γ -valerolactone

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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.

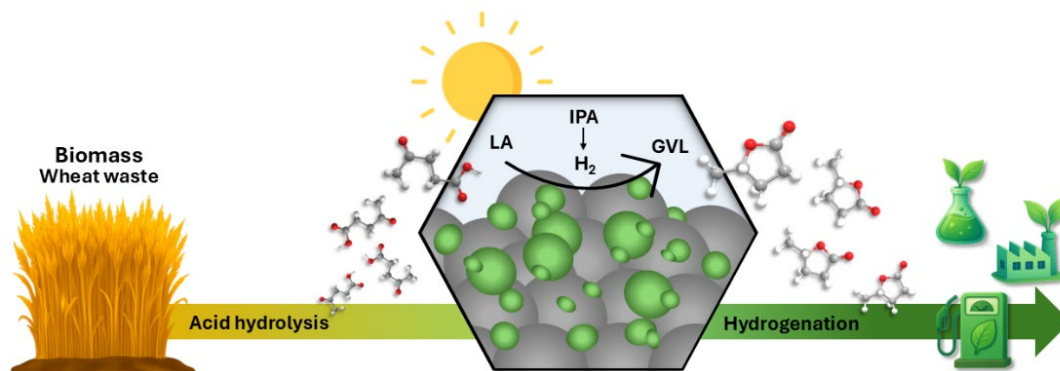


Fig. 1. Schematic representation of the photo-thermocatalytic conversion of levulinic acid to GVL under solar illumination on Ni-based catalysts.

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Entropy management of PLA: Novel state-based screening method for decision-support from feedstock to end-of-life treatment

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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.

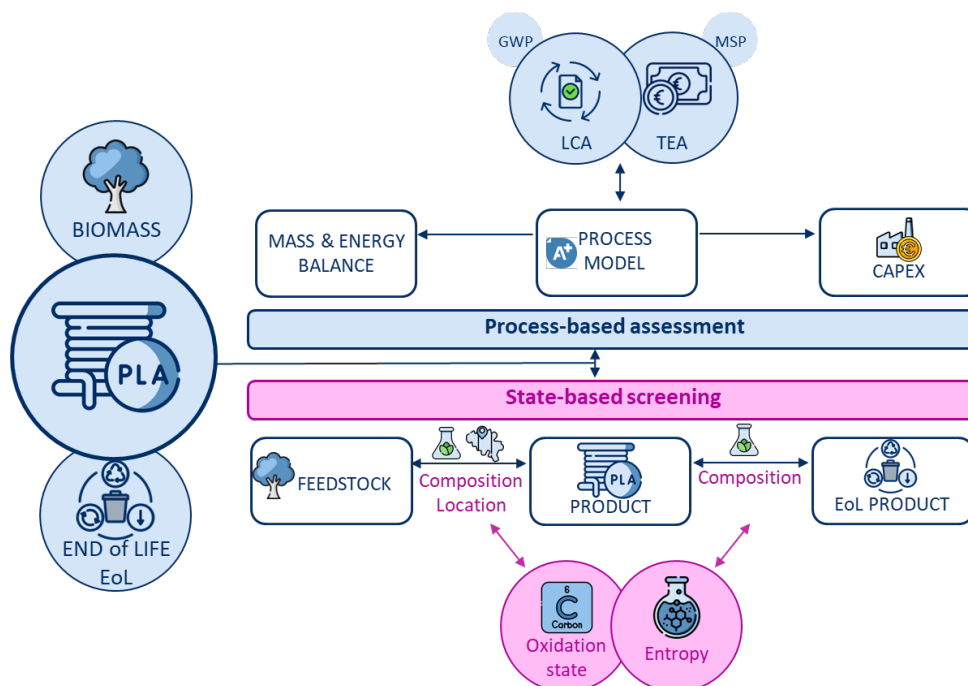


Fig. 2. Introduction of a novel state-based screening method to guide decision-making consistent with process-based assessments applied to the production and end of life of polylactic acid (PLA)

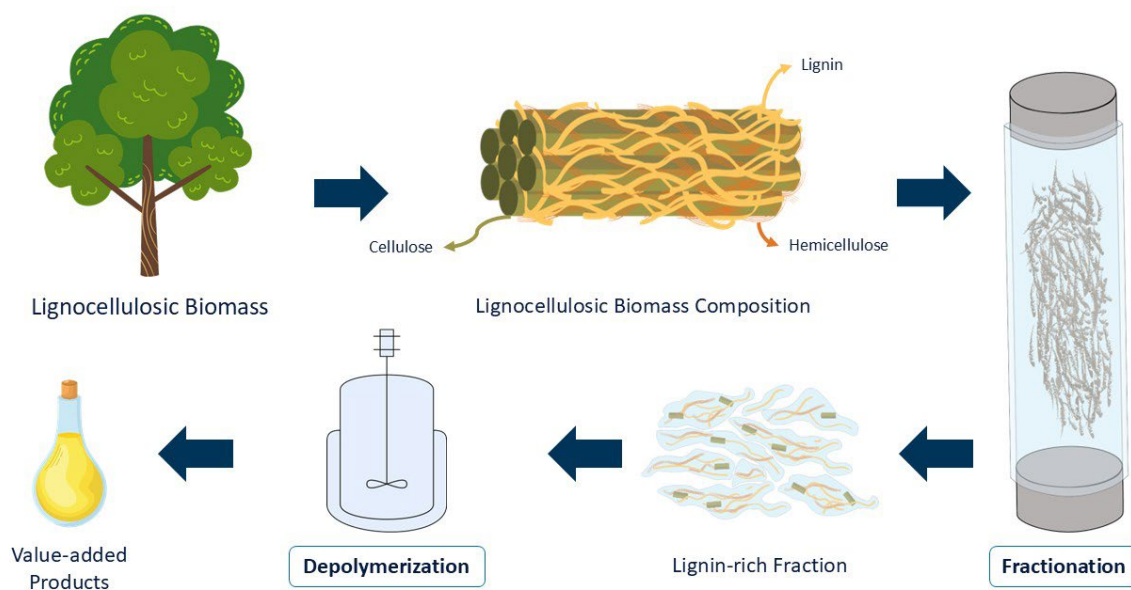
An integrated biorefinery approach for sustainable fuel production via low-pressure flow-through organosolv fractionation and catalytic lignin upgrading

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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/Al₂O₃ 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**

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A mechanically assisted synthesis of ZIF-8¹ 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 m³ H₂/t feed while the inclusion of catalyst in the cracking column lead to the highest yield for H₂.

	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 ₂ S, 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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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 CaCl₂, 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.

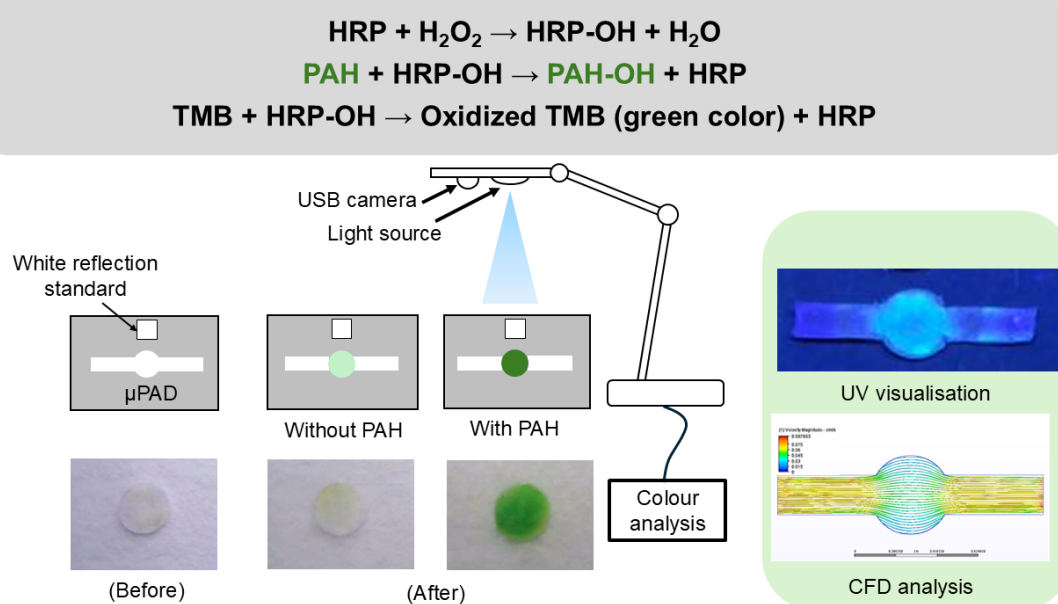


Fig. 1. Experimental set up

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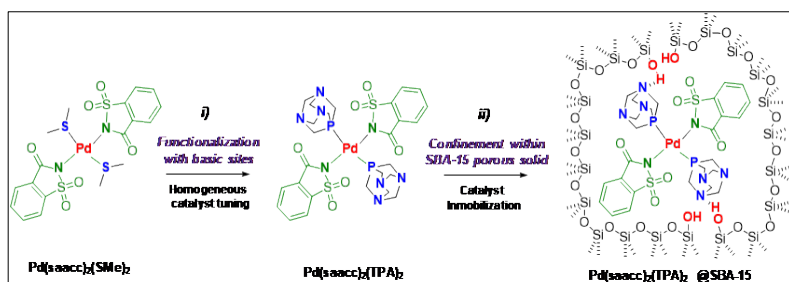
Pd-Imidate@SBA-15: A multifunctional heterogeneous catalyst for the aqueous room temperature hydrogenation of CO₂ to formic acidN. Martín^{1*}, R. Porcar², J.L. Serrano³, J. Pérez³, P. Lozano⁴, F.G. Cirujano^{1*}, E. García-Verdugo^{1*}¹Universitat Jaume I, Spain; ²Universidad Nacional de Educación a Distancia. UNED, Spain; ³Universidad Politécnica de Cartagena, Spain; ⁴Universidad de Murcia, Murcia, Spain

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To reduce CO₂ emissions, thermo-catalytic methods should complement electro- and photocatalytic approaches, which face efficiency and scalability issues. Hydrogenation of CO₂ 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 CO₂ 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 CO₂ hydrogenation to formic acid/formate by forming HCO₃⁻ and CO₃²⁻ species, while the Pd-PTA bond prevents Pd aggregation, and the SBA-15 support improves diffusion, as confirmed by ¹H-NMR and ¹³C-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 CO₂ 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 CO₂ 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 CO₂ valorization.¹Inoue, Y. et al. *Chem. Lett.* **1976**, 5, 863–864.²Martín, N. et al. *ChemSusChem* **2025**, 18, e202401192.

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The European Green Deal sets ambitious targets for greenhouse gas (GHG) emission reduction. Residual, hard-to-abate CO₂ 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 CO₂ 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 CO₂ capture pilot plant for post-combustion capture from diluted industrial flue gases, targeting a capacity of 1 kg CO₂ 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 CO₂ 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.

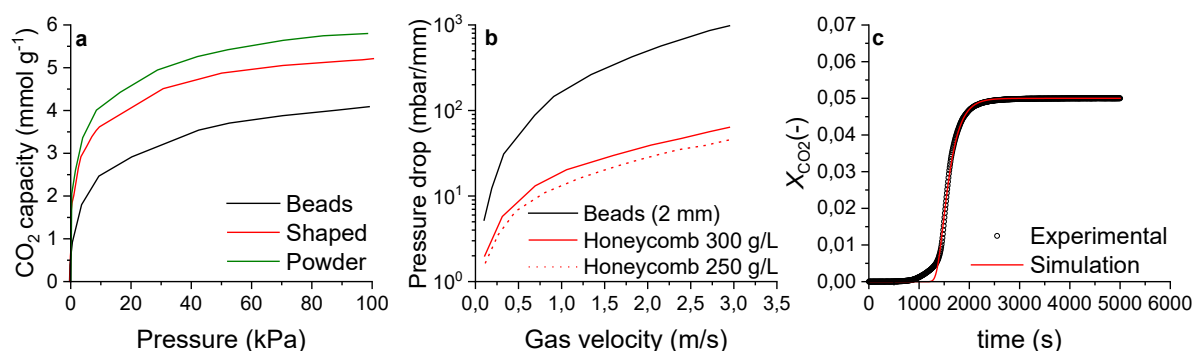


Fig. 3. a) isotherm capacities b) pressure drop measurements and c) dynamic breakthrough experiments.

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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.

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In recent years, studies on microwave-induced CO₂ 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 CO₂ 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 CO₂ conversion and energy cost. The results obtained show CO₂ 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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The catalytic reduction of CO₂ into value-added chemicals using renewable energy is a promising strategy for effective CO₂ management. However, the competing hydrogen evolution reaction (HER) significantly hinders the reaction's efficiency and product selectivity. Herein, Zr₁₂O₁₂ and M@Zr₁₂O₁₂ (M = Fe, Co, Ni, Cu, Zn) nanocages have been investigated for the photocatalytic CO₂ reduction reaction (CO₂RR) using first-principles calculations. It was observed that Fe, Co, and Ni atoms are stable on the Zr₁₂O₁₂ 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 Zr₁₂O₁₂ is significantly reduced to 2.07 eV, which is further decreased upon loading with Fe, Co, and Ni. Notably, pristine Zr₁₂O₁₂ can convert CO₂ to CO under a relatively low potential of 0.71 eV. However, the desorption of CO from Fe@Zr₁₂O₁₂, Co@Zr₁₂O₁₂, and Ni@Zr₁₂O₁₂ nanocages is thermodynamically unfavorable due to large energy barriers. Interestingly, the Ni@Zr₁₂O₁₂ nanocage can spontaneously reduce CO₂ to OCCO, an important intermediate in the formation of C₂ products. But unfortunately, the strong binding energy of H atom on Ni@Zr₁₂O₁₂ may block active sites, thereby hindering the CO₂RR. In contrast, Zr₁₂O₁₂, Fe@Zr₁₂O₁₂, and Co@Zr₁₂O₁₂ can form OCCO intermediates under external energies of 0.71, 0.67, and 0.69 eV, respectively. Moreover, Fe@Zr₁₂O₁₂ and Co@Zr₁₂O₁₂ nanocages exhibit stronger CO₂ adsorption than H adsorption, which may favor the CO₂ reduction reaction.

Keywords: Zr₁₂O₁₂ nanocage; single-atom catalyst; CO desorption; C-C coupling.

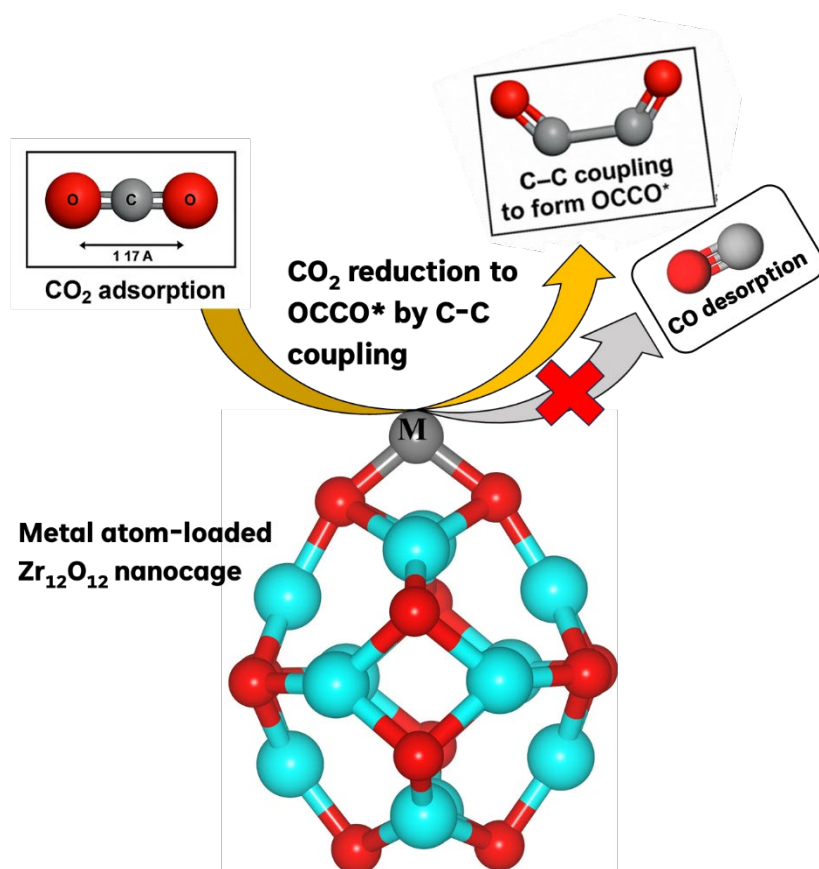


Fig. 1. C–C coupling reaction on the metal-loaded Zr₁₂O₁₂ nanocage.

Rapid mechanosynthesis of carbon-doped nickel sulfides for efficient evolution of hydrogen via water splitting

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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 -Ni₇S₆, and Ni₃S₂ was produced. The reaction was completed in about ten seconds. Increasing carbon content shifted the phase composition, decreasing the intensity of α -Ni₇S₆ 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 $\mu\text{F}\cdot\text{cm}^{-2}$ to 10.61 $\mu\text{F}\cdot\text{cm}^{-2}$ 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.

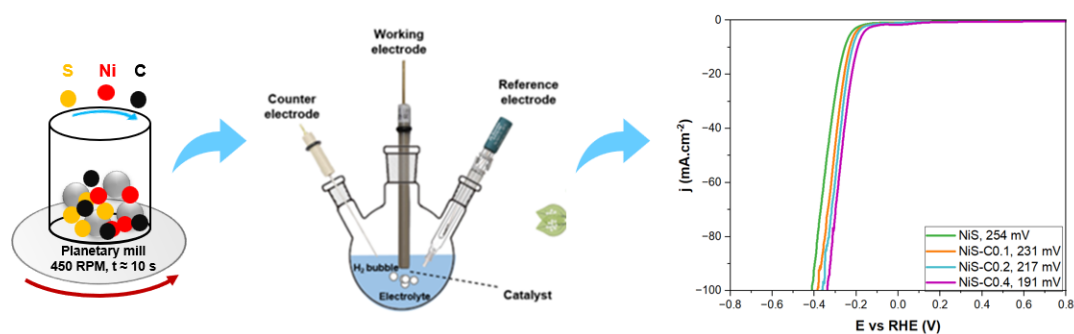


Fig. 1. Synthesis and electrocatalytic performance of nickel sulfide electrocatalysts

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Silica coating of PEM fuel cell Pt/carbon electrocatalysts to enhance durability upon operation

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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 efficiency¹.

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 properties⁴.

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.

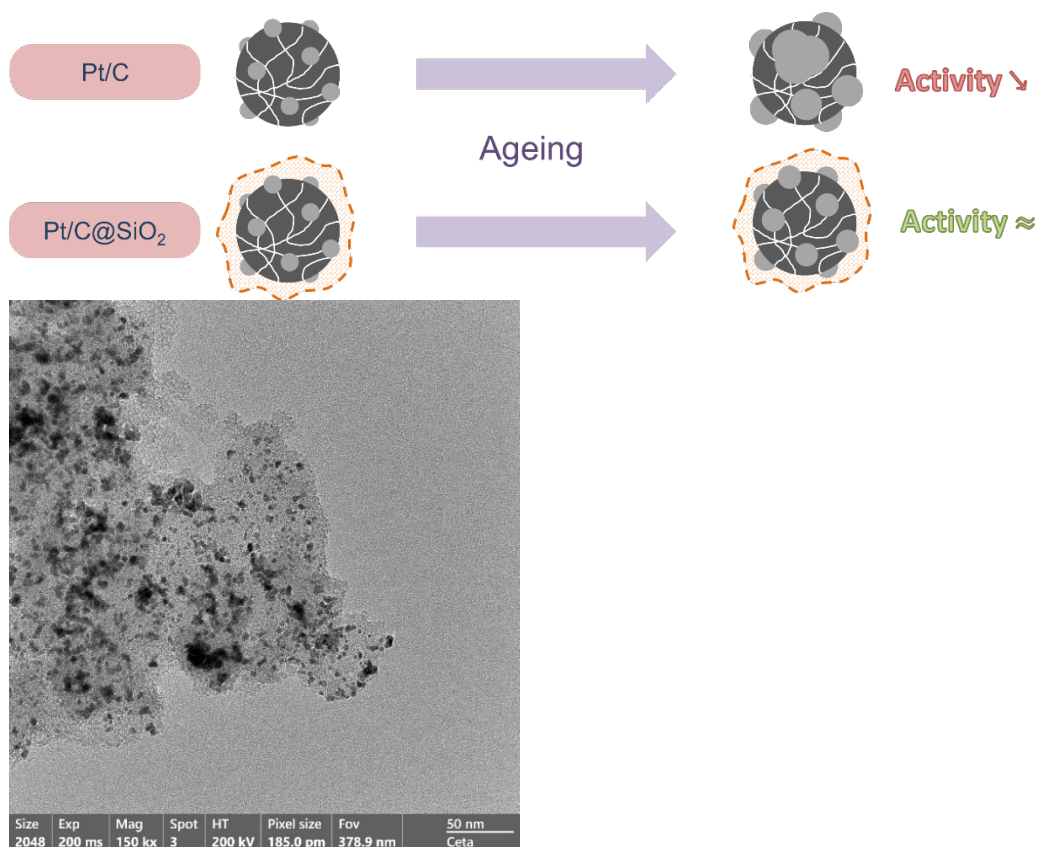


Fig. 1. (up) Goal of the project and (bottom) TEM image of a Pt/CX sample covered by a silica layer

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Improved chemical recycling of PET derivatives: Enhanced glycolysis via morphology control and catalysisChang joon Park¹, Geon kyo Park¹, 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.

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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, BiVO₄ 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 BiVO₄ 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 BiVO₄, 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 transportation 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 BiVO₄ 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.

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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 WPCBs 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 $\text{H}_2\text{SO}_4\text{--CuSO}_4\text{--NaCl}$ 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.

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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 $\text{H}_2\text{SO}_4\text{--CuSO}_4\text{--NaCl}$ 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.

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Antiviral Co-doped ZnO pigments: Solution combustion synthesis using *Aloe Vera* extract as an alternative green fuel

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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 ZnCo₂O₄ (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).

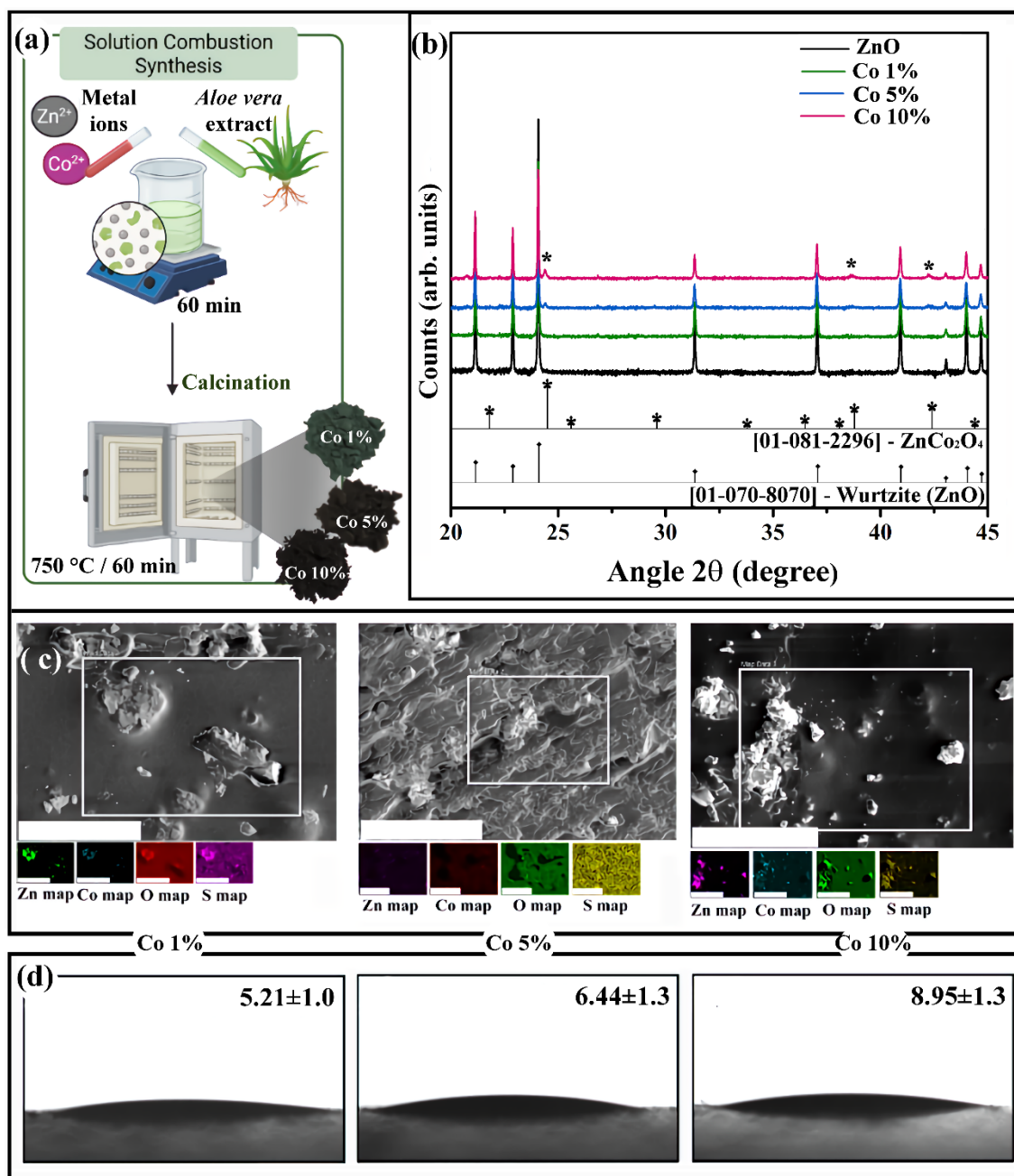


Fig. 4. (a) Schema of the SCS utilized in this study at 750 °C, with varying concentrations of the dopant ion (1%, 5%, and 10% by mass relative to Zn ions); (b) X-ray Diffraction (XRD) patterns of the synthesized pigments, with the spinel phase of ZnCo₂O₄ indicated by an asterisk (*) in the image; (c) 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 (%)
Polycarbonate (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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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 m²/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.

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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.

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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 materials¹.

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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Supporting environmental remediation through the NanoEnviCZ infrastructure: Development of cyclodextrin-modified nanofibrous membranes

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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.

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Establishing Raman spectral references for climate- and energy-relevant materials through *ab initio* dynamics and experimental tools

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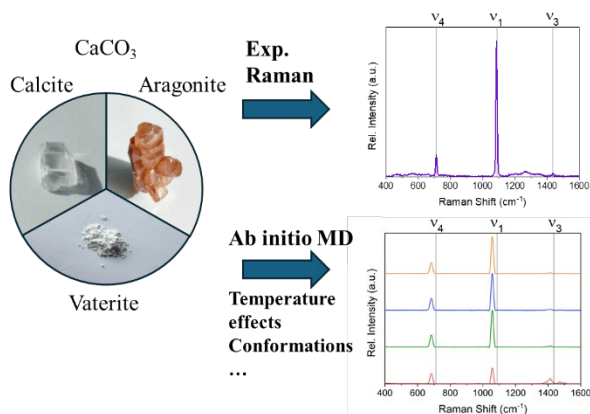
Establishing precise reference data that enables the use of green characterization techniques is essential for advancing sustainable materials science. In this context, theoretical spectroscopy has demonstrated strong capabilities, with dynamic Raman spectroscopy offering a powerful computational framework 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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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 pathways¹. 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.

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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/SnO₂ 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 SnO₂/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/SnO₂ 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.

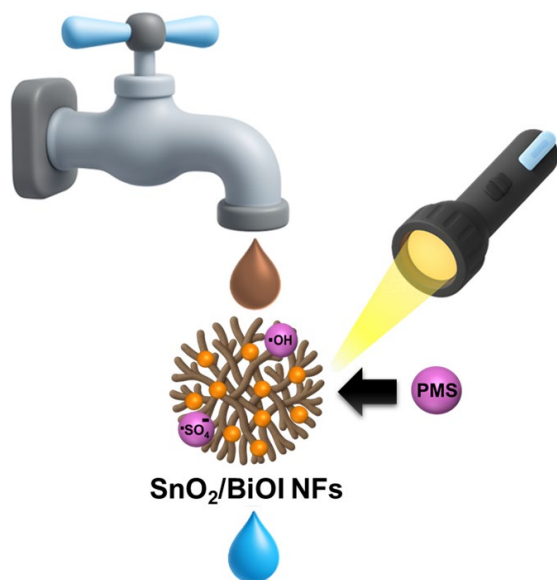


Fig. 5. Schematic illustration of visible-light/PMS-activated multipollutant degradation over electrospun SnO₂/BiOI nanofibers.

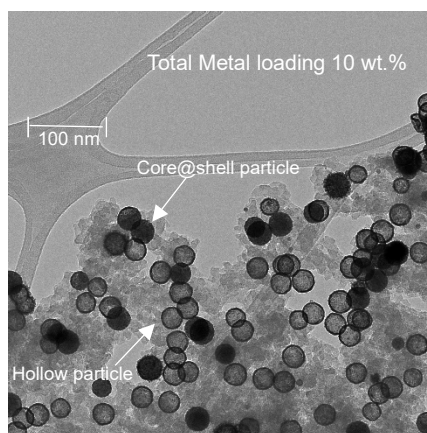
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Development of hollow bimetallic catalysts supported on nanostructured carbons for sustainable PEM fuel cell electrodesAli Haider^{1,2}, Lucas Elvira², Loïc Noumbi¹, Sophie Hermans², Nathalie Job¹¹University of Liège, Dept. of Chemical Engineering (B6a), Belgium; ²UCLouvain, 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 degrade²: 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 slowly³. Alloying Pt with transition metals such as Co or Ni contracts the Pt lattice, which reduces the binding energy of oxygen reduction intermediates⁴. 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 work³, 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 HClO₄, exhibiting higher mass and specific activities than commercial Vulcan Pt/C material.

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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 demand¹. Conventional water treatment methods, such as chlorination and ultraviolet irradiation, are effective but may generate harmful disinfection byproducts and contribute to bacterial resistance². 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 methods⁴. 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 nanoparticles⁵. 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-H₂O, 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.

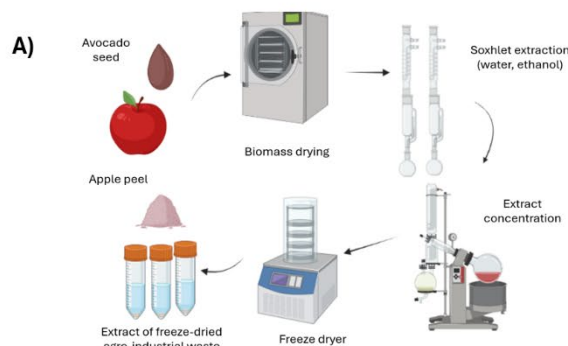


Fig 1. Process for obtaining extracts from agro-industrial residues

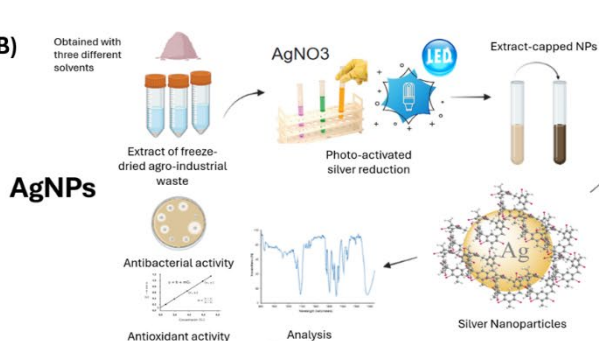


Fig 2. Synthesis of silver nanoparticles under LED light

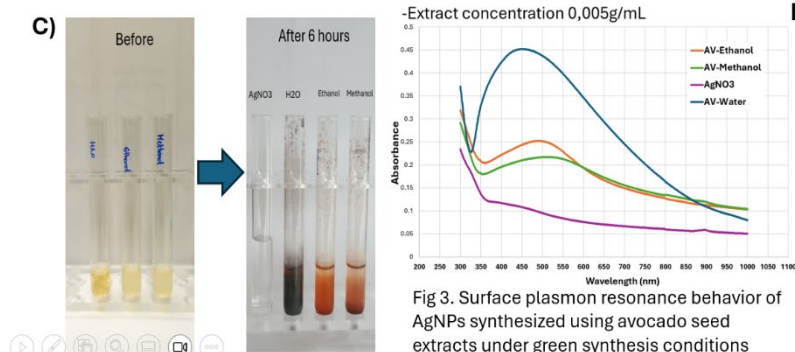


Fig 3. Surface plasmon resonance behavior of AgNPs synthesized using avocado seed extracts under green synthesis conditions

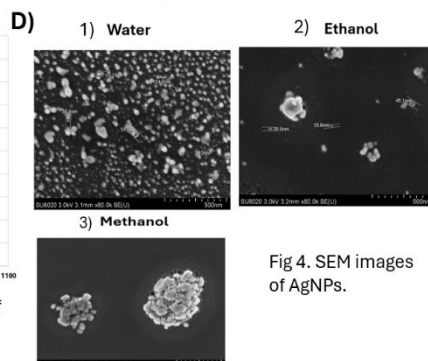


Fig 4. SEM images of AgNPs.

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).

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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).

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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.

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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.

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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 Σ PFAS, 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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Toward sustainable aromatics production: Zeolite-catalyzed conversion of biomass- and CO₂-derived alcohols

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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 CO₂ 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 stability³. 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.

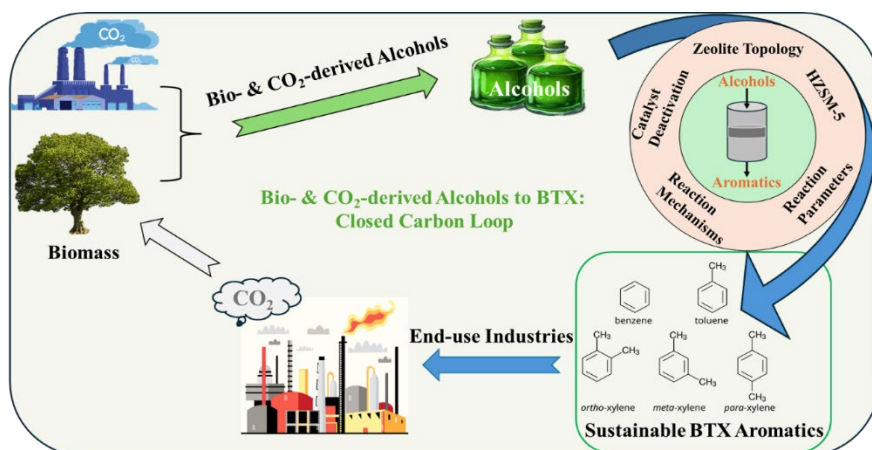


Fig. 6. Closed-carbon pathway from biomass/CO₂-derived alcohols to sustainable BTX aromatics.

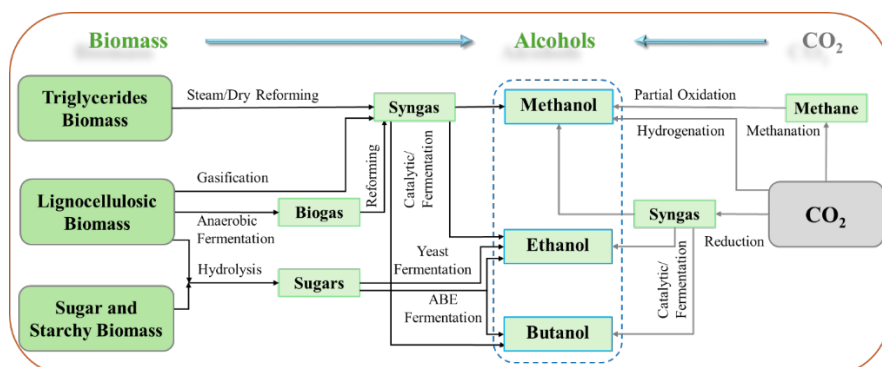


Fig. 7. Schematic representation of renewable alcohol production from biomass and CO₂ feedstocks.

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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The continuous rise in atmospheric carbon dioxide (CO₂), 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 CO₂ valorization strategies which transform this abundant greenhouse gas into different value-added chemicals. In this context, the catalytic hydrogenation of CO₂ 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 CO₂ hydrogenation. This disparity can be attributed to the comparatively lower hydricity character and greater thermodynamic stability of Rh–H bonds, which disfavor the key CO₂ 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 CO₂ 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 CO₂ hydrogenation but also provide new design principles for developing efficient hydrogenation catalysts based on alternative ligand–metal architectures.

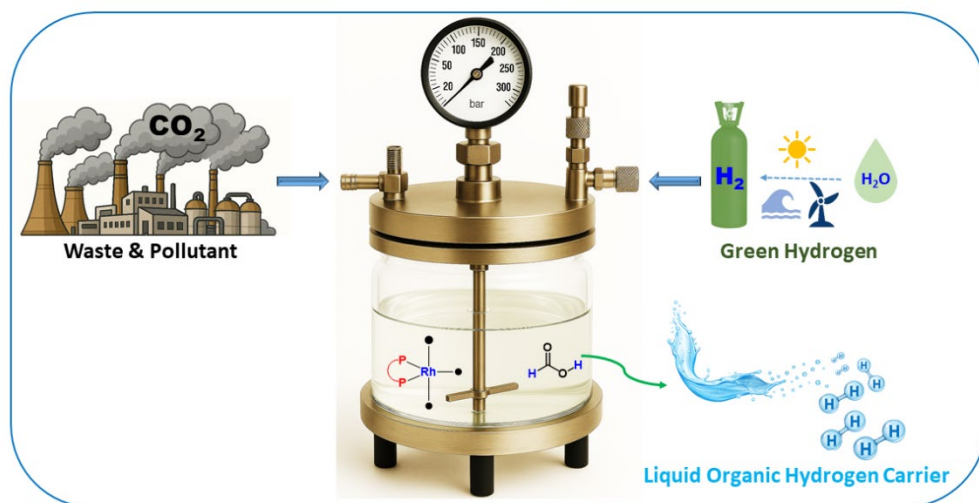
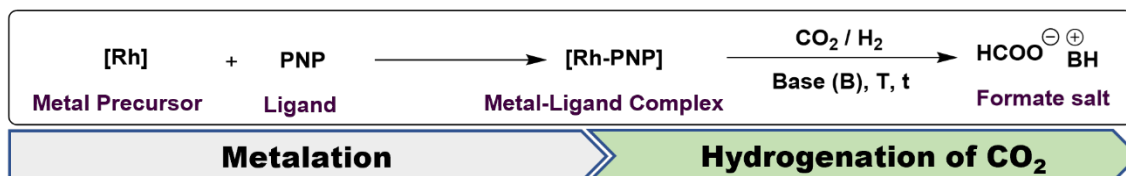


Image 1. Overview of the Significance of the Present Study

Image 2. One-top Strategy for CO₂ Hydrogenation to Formate¹Roy B.C., Jaseer EA, Mousa A.H., Maity N. *Renew. Sustain. Energy Rev.* **2026**, 226, 116371.²Eppinger J, Huang K-W. *ACS Energy Lett.* **2017**, 2, 188.

Closed-loop chemical recycling of PET via glycolysis: Preserving structural, thermal, and molecular integrity with post-consumer wasteZulfiqar Ahmed Rehan¹, Saqib Nasib Rana¹, Imran Hassan Syed¹¹Dept. 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 ¹H 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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Polyethylene terephthalate (PET) is one of the most daily used plastics in the world. 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.

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The hydrogenation of CO₂ 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/Ti₂C@Ti₂O₅ catalyst that exploits a strong electronic metal–support interaction (EMSI) enabled by a Ti₂C 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 CO₂ activation. Adsorption studies using H₂-TPD and CO₂-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 CO₂ 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

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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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Upgrading date palm-derived organosolv lignin oil into cycloalkanes for sustainable aviation fuel (SAF) via Ni-based bifunctional catalysis

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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°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°C) to obtain deoxygenation as high as 90%, towards respective C6-C9 alkyl-aromatic and cycloalkanes.

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EES - D1- P65

Ni/LaMnO₃ perovskite catalysts promoted by alkali and alkaline earth metals for green hydrogen generation via NH₃ decomposition

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Chemical hydrogen carriers such as ammonia (NH₃) have garnered increasing attention. NH₃ 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 CO₂-free, on-demand hydrogen production.

In this study, LaMnO₃ 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, H₂-TPR, and CO₂-TPD) confirmed the successful integration of promoter elements without compromising the perovskite structure. NH₃ 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% NH₃/He, H₂, and He), and an online GC.

Catalytic testing revealed that unpromoted Ni/LaMnO₃ achieved 90% NH₃ conversion only at 640 °C, highlighting the need for further enhancement. Among all samples, the 3%K-Ni/LaMnO₃ 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/LaMnO₃ > 3%Cs-Ni/LaMnO₃ > 3%Sr-Ni/LaMnO₃ > 3%In-Ni/LaMnO₃ > 3%Ca-Ni/LaMnO₃ > Ni/LaMnO₃, and these results elucidate the critical role of K in enhancing the performance of Ni/LaMnO₃ catalysts.

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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., $\text{Mo}_2\text{Ti}_2\text{AlC}_3$) 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 $\text{Mo}_2\text{Ti}_2\text{C}_3$** , 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.



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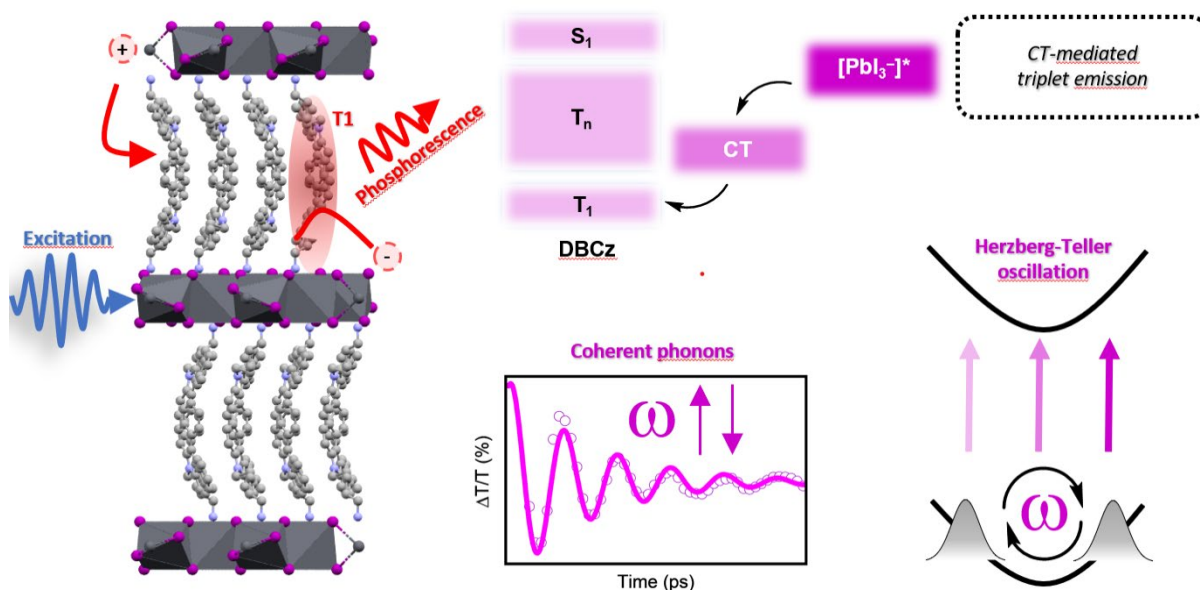
IM - D1 - P04

Ultrafast charge transfer and coherent phonons in electroactive organic cation-templated low-dimensional perovskite analogues

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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)₂PbI₄, and a previously unreported layered perovskite analogue structure with edge-sharing octahedra, DBCzPbI₃. 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.



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IM - D1 - P05

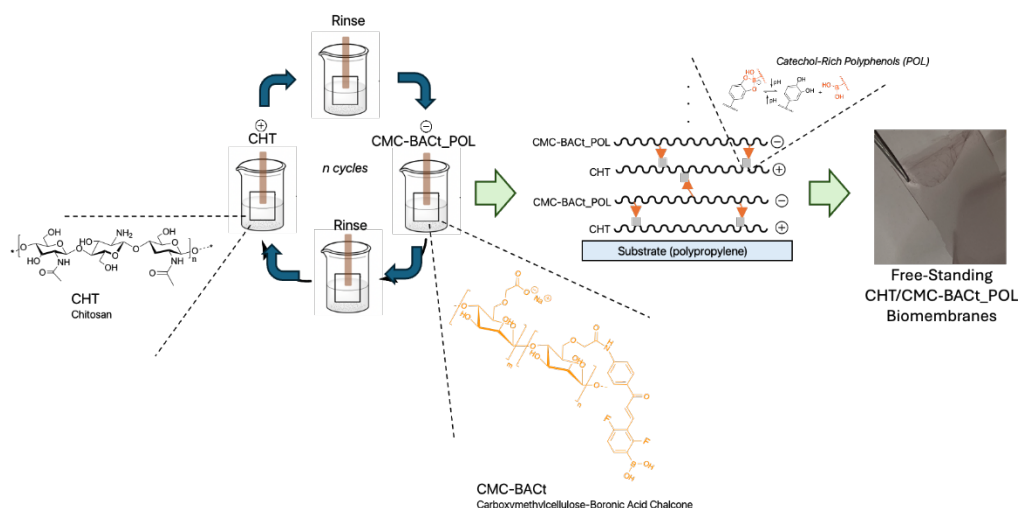
Layer-by-layer supramolecular assembly of boronic acid chalcone-containing biomembranes for pH-controlled complexation of catechol-rich polyphenols

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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.

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IM - D1 - P06

Ti-based core-shell shaping for Ac-225/Bi-213 separation

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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** ($\geq 80\%$ ^{213}Bi yield in 2 mL eluate), is needed. Moreover, the harsh separation conditions—exposure to highly acidic medium ($< \text{pH } 3$) 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.

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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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Almudena Terrel, Mauricio Vera-Arévalo, Alberto Concellón

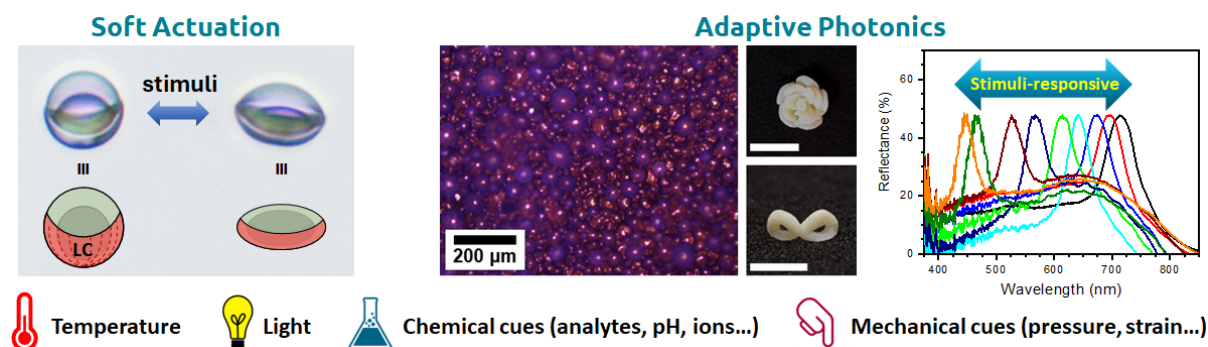
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Liquid crystal (LC) emulsions have emerged as highly versatile soft matter systems in which interfacial geometry and molecular order can be precisely engineered to access a wide range of adaptive functionalities.¹ By combining the dynamic morphologies 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.



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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.

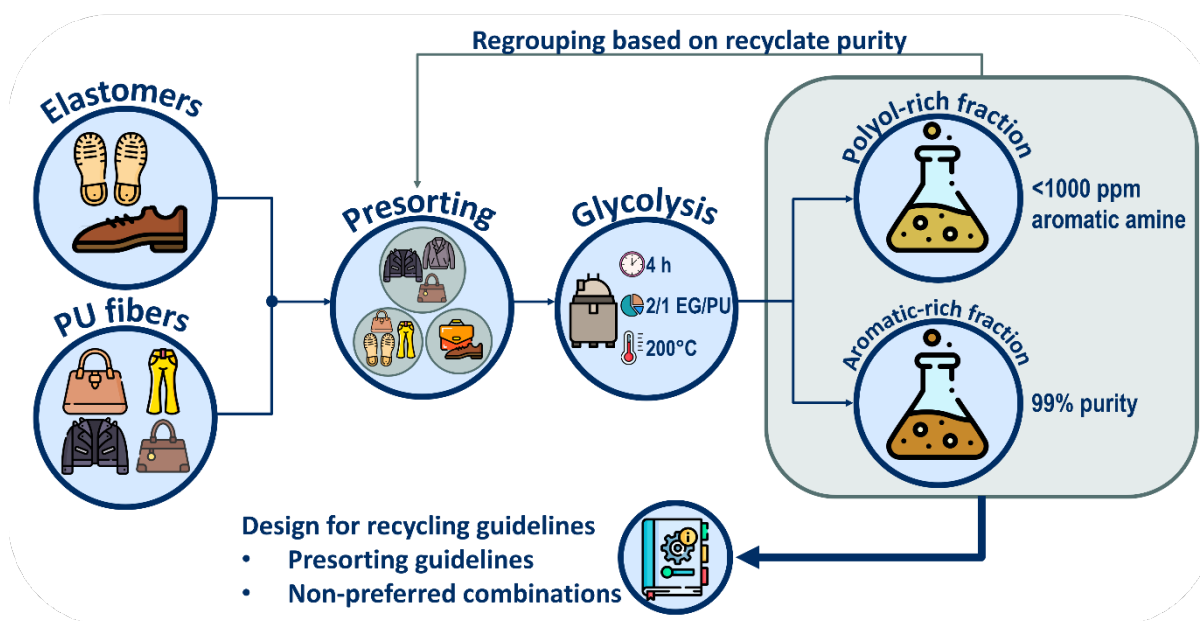


Fig. 1. Applicability of flexible-foam glycolysis to diverse and complex PU waste streams

Tzu Hsuan Chiang^{1*}, I-Chia Yang¹¹*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.

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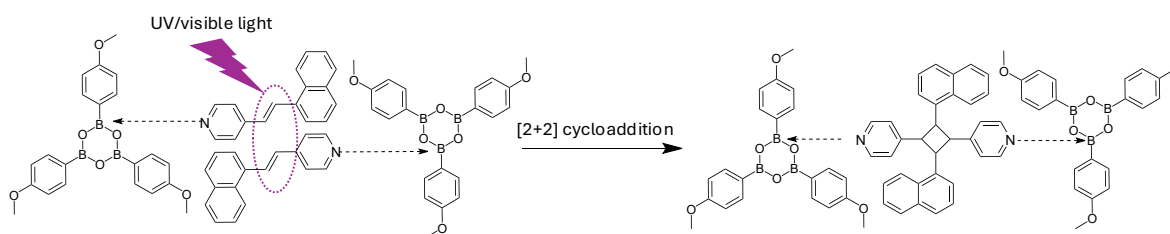
IM - D1 - P11

Structural mapping of photosalient B←N molecular crystals featuring intermediary dimer clusters

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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

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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 $^{225}\text{Ac}/^{213}\text{Bi}$ 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 $\text{pH} \geq 3$ 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.

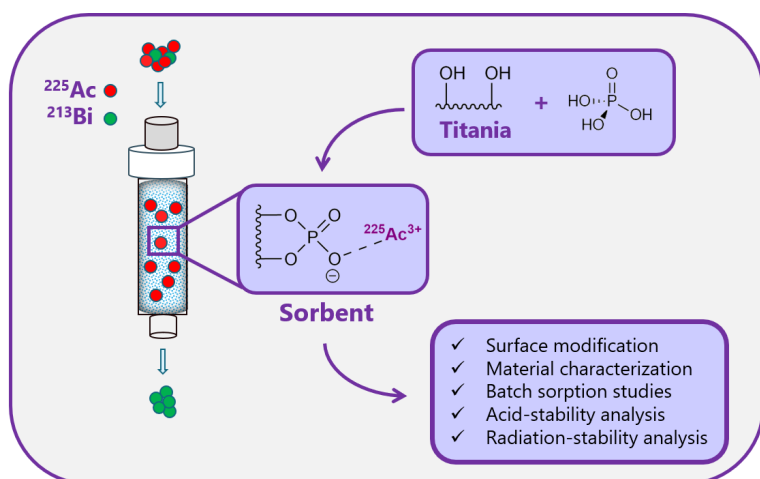


Fig. 2. Visual representation of research

Corentin Pochet, Catherine Aitchison

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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.

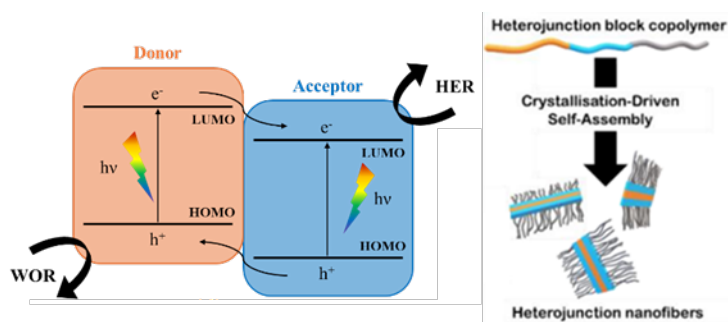


Fig. 3. Schematic of D-A heterojunctions and CDSA of nanofibers.

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IM - D1 - P14

Stability enhancement of polyetherimide under harsh space conditions via covalently bound self-passivating silica layers

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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 robustness¹. However, prolonged exposure to galactic cosmic rays, solar wind, and/or atomic oxygen causes erosion, mass loss, and deterioration of mechanical, thermal, and electrical properties². Inorganic barriers (e.g. SiO₂, Al₂O₃, ZrO₂) 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 functionalization³: 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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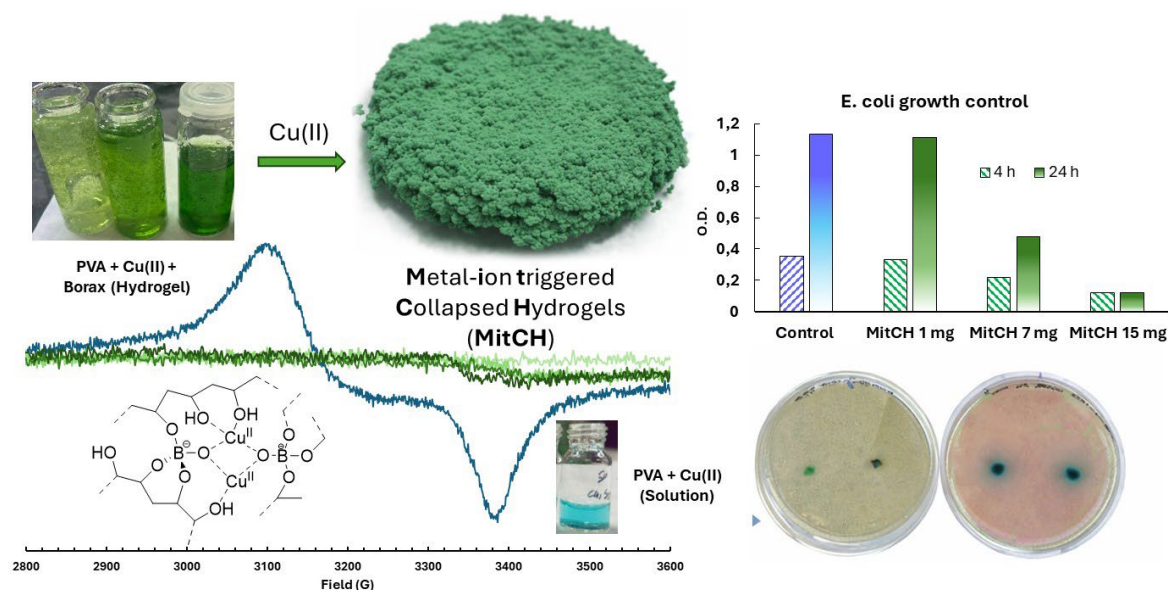
IM - D1 - P15

Metal ion-triggered collapsed hydrogels as new materials for bacterial population control

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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

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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.

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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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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 mass¹. 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 pollution². 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 synthesis².

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 reactions³. 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 $\text{Mn}^{3+}/\text{Mn}^{2+}$ and $\text{Ni}^{3+}/\text{Ni}^{2+}$ oxidation states⁵. 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 phases⁸. The absence of distinct Mn or Ni peaks indicates successful incorporation of the dopant ions into the H-Ap or β -TCP crystal structures⁹, confirming effective waste-derived pigment synthesis with strong anticorrosive potential.

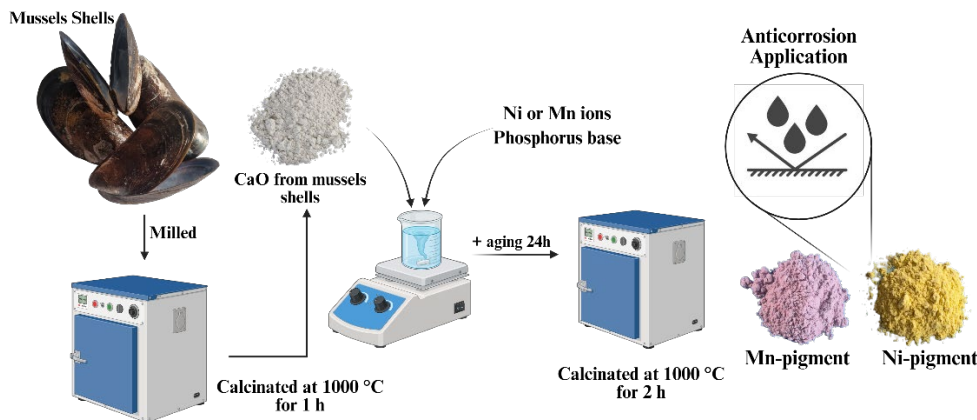


Fig. 1. Pigment synthesis schema: The synthesis was performed via a wet-chemical route. In the first stage, the mussel shells were milled and thermally treated to produce CaO. In the second stage, the reagents were dispersed in 50 mL of deionized water and homogenized under magnetic stirring for 2 hours. 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.

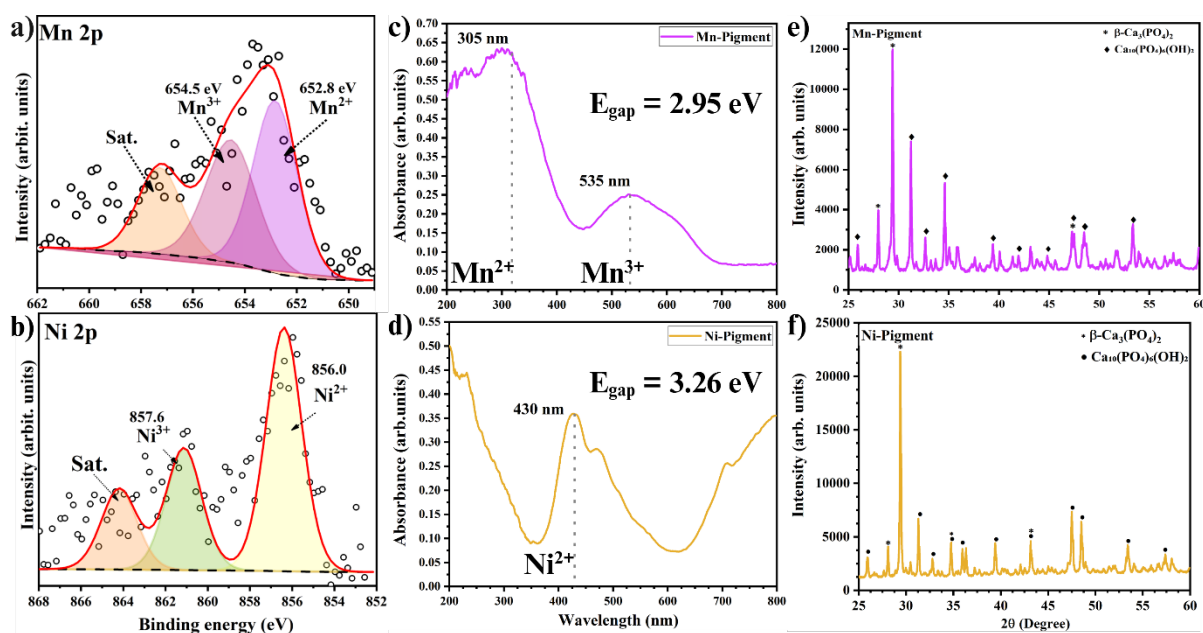


Fig. 2. Spectrum XPS for the (a) Mn-pigment and (b) Ni-pigment, where the binding energies were calibrated using the C1s peak (284.6 eV) as a reference. The detection of synthesized (c) Mn-pigment and (d) Ni-pigment was done in UV–UV-visible spectrophotometer by scanning the absorbance spectra in the range of 200–800 nm. The crystalline structure of the (e) Mn-pigment and (f) Ni-pigment was characterised by XRD, with a CuK α radiation source of $\lambda = 1.5418 \text{ \AA}$, potential of 40 kV, current of 30 mA, varying between 25–60° (2 θ), 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

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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 storage¹. 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) salt². 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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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.

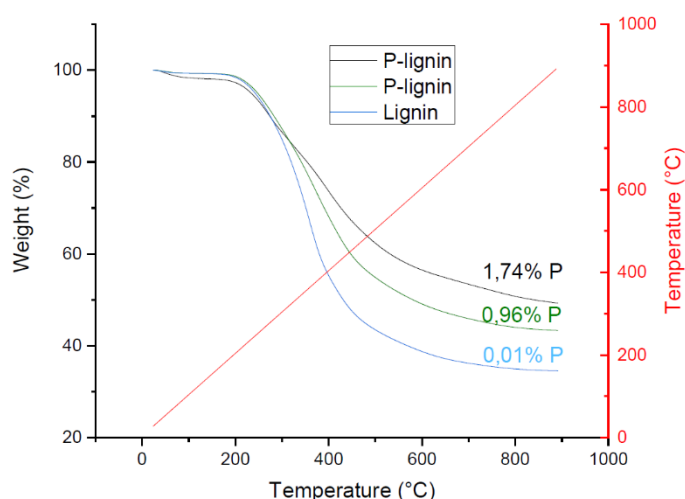


Fig. 4. Thermal gravimetric analysis (TGA) of a kraft lignin residue (Lignin) and two modifications enriched in phosphorus.

Engineering indenofluorenes with controlled diradical character and excited-state aromaticity toward singlet fission

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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.

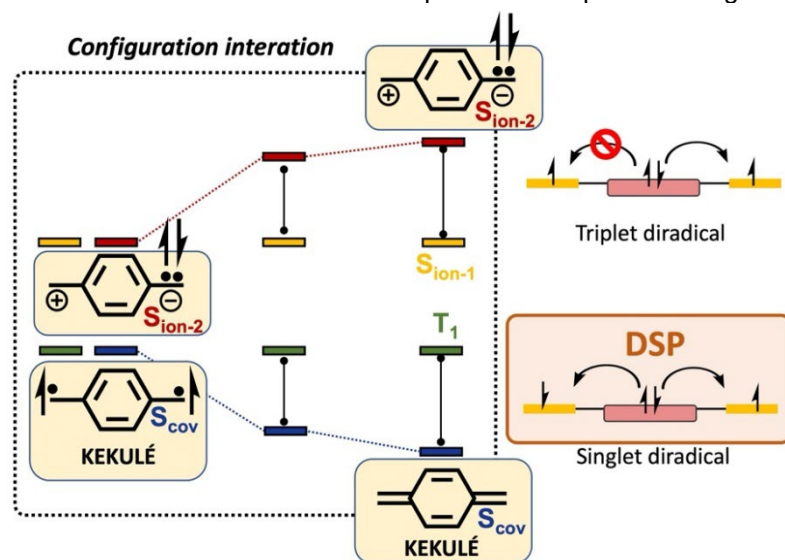


Fig. 1. Representation of how mixing between the covalent ground-state configuration and the ionic configurations modulates the energy distribution of the excited states, together with the double spin polarization (DSP) mechanism that stabilizes the singlet configuration relative to the triplet.

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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 (γ CD) 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 γ CD 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 $\tan\delta < 1$ 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.

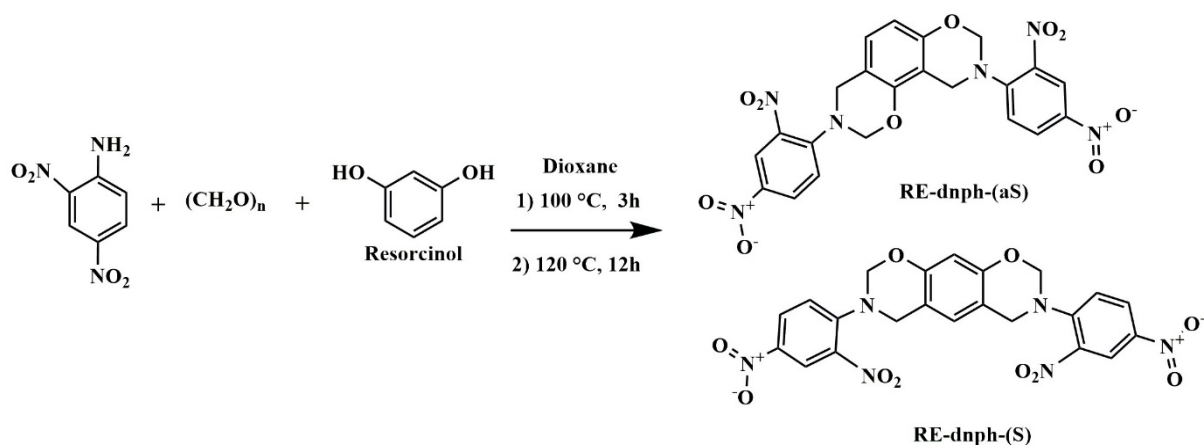
Table 1. Rheological results of hydrogels.

Gel	η (Pa.s)	Max G' (Pa)	$\tan\delta$	Gelation T (°C)	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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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·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 ₈ O ₁₀
Molecular weight (g·mol ⁻¹)	554
Appearance	Reddish powder
Heat of combustion -ΔU _{comb} (kJ·g ⁻¹)	23.33
Enthalpy of combustion -ΔH _{comb} (kJ·mol ⁻¹)	1775.82
Heat of formation -ΔfH (kJ·mol ⁻¹)	9466.18
Oxygen balance OB (%)	-124.18

Deflagration temperature T _{def} (°C)	261
Density ρ (g·cm ⁻³)	1.59

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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-trifluoromethanesulfonimide (NTf₂⁻) 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.

Interfacial effects of monomeric and dimeric surfactants in waste-oil microencapsulation for advanced self-healing materials

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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.

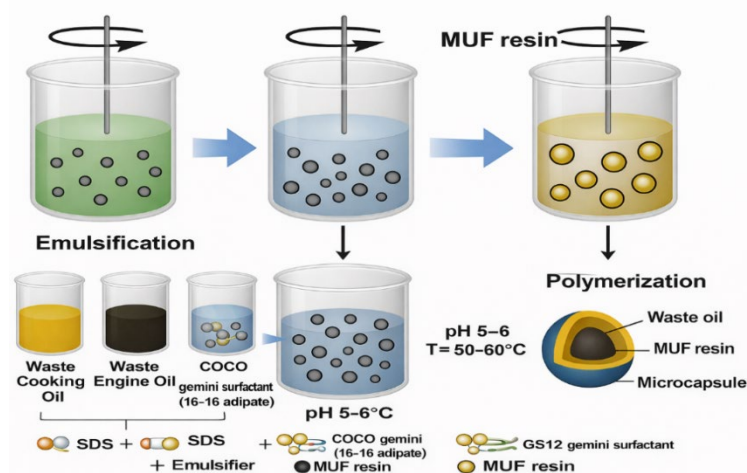


Fig. 1. Schematic of the synthesis process of microcapsules containing WCO and WEO by in situ polymerization.

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Molecular Design & Reactivity (MDR)

MDR - D1 - P01

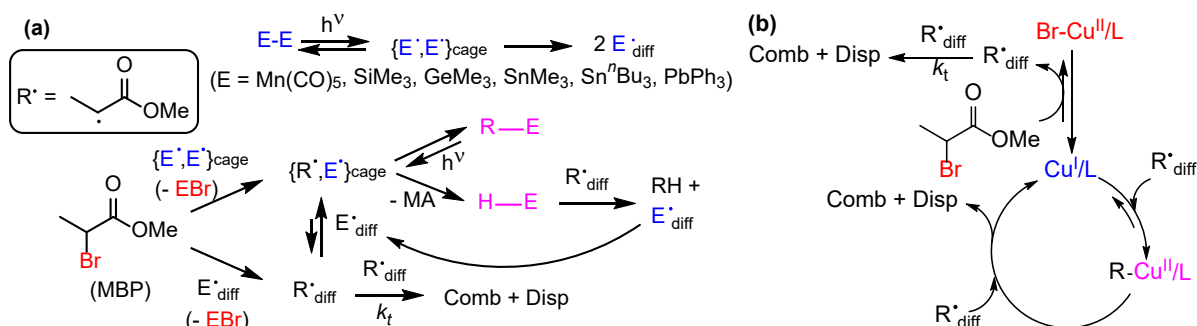
How do acrylate radicals terminate? New evidence to settle a never-ending debate

Laurianne Forget¹, Krzysztof Matyjaszewski,² Christophe Fliedel,¹ Rinaldo Poli¹

¹Laboratoire de Chimie de Coordination (LCC CNRS), CNRS, Université de Toulouse, France; ²Dept. 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, $\cdot\text{CH}(\text{Me})(\text{COOMe})$, generated by Br-atom abstraction from methyl 2-bromopropionate (MBP) by either a stronger heteroatom radical, $\text{E}^\cdot$, obtained by photolysis of stable E-E precursors ($\text{E} = \text{Mn}(\text{CO})_5$, 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 $\text{E}^\cdot$ 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.



Funding by project ANR-23-CE06-0001-01 is gratefully acknowledged.

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MDR - D1 - P02

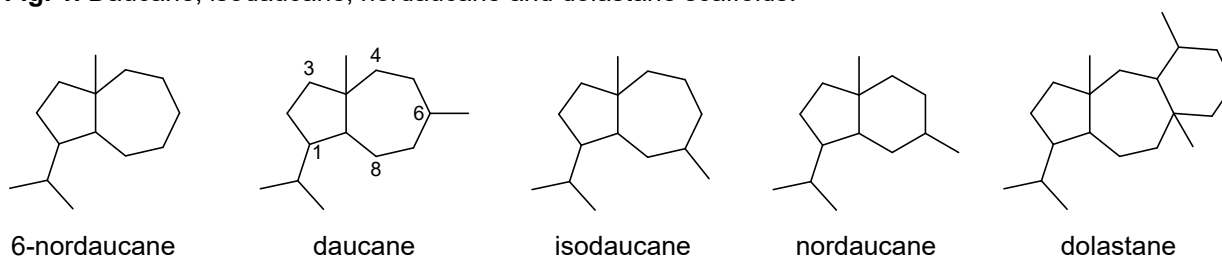
Verification, falsification and revision of the constitution and configuration of daucane sesquiterpenoids based on total synthesis and X-ray crystallography

Josefine Brindöpke¹, Adrian Dennis Podlesny¹, Martin Hiersemann¹

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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.



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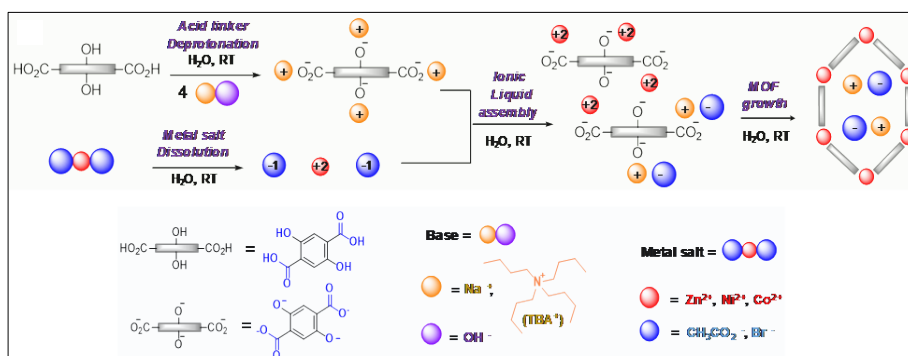
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This study introduces a green, one-pot synthesis for incorporating ionic liquids (ILs) into metal-organic frameworks (MOFs) to enhance CO₂ fixation. By using strong bases and metal bromides in water, the method eliminates toxic solvents and enables 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 CO₂-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 CO₂ 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@M₂(dot) ionic-liquid/MOF hybrid materials can promote the CO₂ 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 CO₂ (balloon).



Scheme 1. Design of MOF-ILs as catalysts for CO₂ fixation into carbonates.

¹Martín, N. et al. *NanoResearch* **2025**, *18*, 94907069.

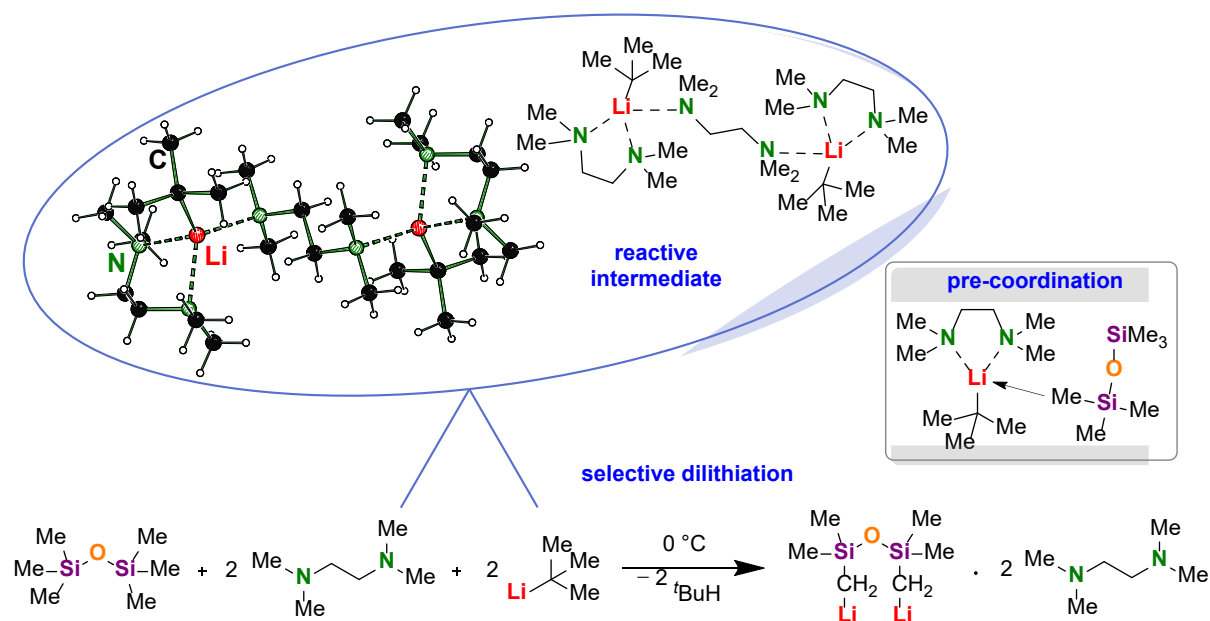
Why can we deprotonate methylsiloxanes with the combination of *t*-BuLi and TMEDA?Mara Schöler¹, Johannes Kleinheider¹, Tristan Mairath¹, Rebecca Scheel¹, Carsten Strohmann¹¹Faculty of Chemistry and Chemical Biology, TU Dortmund University, Germany

Alkyl lithium 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 alkyl lithium 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 alkyl lithium 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.

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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.

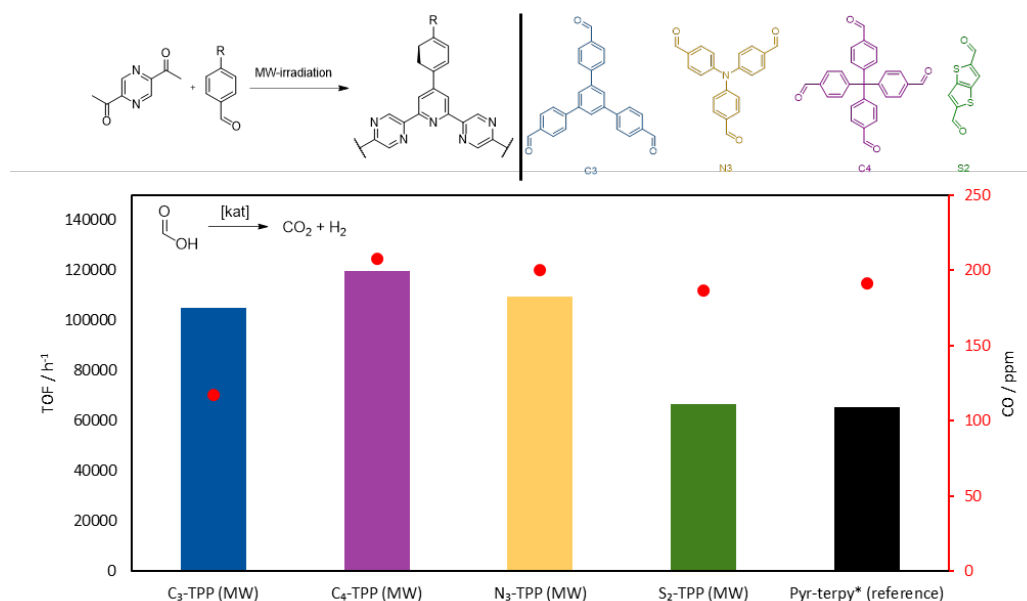


Fig. 1. Synthetic pathway and aldehyde scope of microwave terpyridine polymer (TPP) materials with formic acid dehydrogenation results, including TOF and CO content. Parameters: 15 mg catalyst (1 wt% Ir), 6 mL formic acid solution (10 wt%), 160 °C, 750 rpm, 1 h in Hastelloy steel autoclaves.

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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Márk Váradi¹, Mátyás J. Gazsi¹, Lajos Fodor¹, Rita Skoda-Földes¹¹University 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 molecules³ or strong acids,⁴ terpyridine analogue **L** (Figure 1) with ferrocenylpyrimidine moieties was synthesised starting from ferrocenecarboxaldehyde. Formation of ML₂- and ML-type complexes upon the addition of triflate or acetate salts of various metals (Cu²⁺, Zn²⁺ and Fe²⁺) 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 ZnL₂ 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, Cu²⁺ can displace Zn²⁺, Fe²⁺ or Ag⁺ ions, and this can be traced by cyclic voltammetry. Consequently, the ferrocenyl ligand makes it possible to detect Cu²⁺ ions even in the presence of other metals.

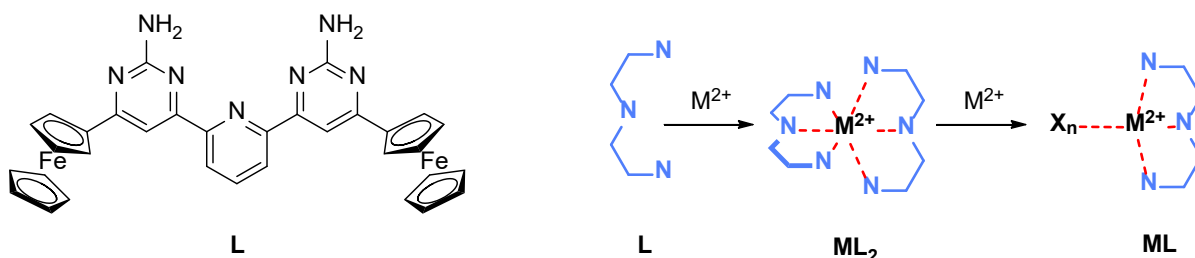


Fig. 1. Ferrocenylpyrimidine ligand **L** and formation of its metal complexes

The financial support of the National Research, Development and Innovation Office (Project: Advanced 149644) is acknowledged.

¹Kainat, S. F. et al. *RSC Adv.*, **2024**, *14*, 21464-21537.

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⁴Keszei, S.J. et.al, *Micropor. Mesopor. Mater.* **2020**, *308*, 110380

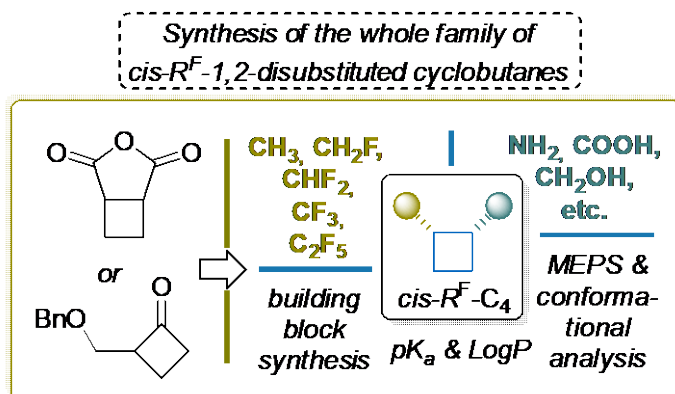
Synthesis and physicochemical assessment of *cis*-R^F substituted cyclobutane derivatives

Oleksandr Liashuk^{1,2}, Anton Chernykh^{3,4}, Kyrylo Kononenko³, Artem Michuda^{2,3}, Oleksandr Olifir^{3,5}, Serhiy Ryabukhin^{1,2,3}, Dmytro Volochnyuk^{1,3,4}, Oleksandr Grygorenko^{1,2,3}

¹Enamine SRI, Ukraine; ²Taras Shevchenko National University of Kyiv, Ukraine; ³Enamine Ltd., Ukraine;

⁴Institute of Organic Chemistry NASU, Ukraine; ⁵V. P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry NASU, Ukraine

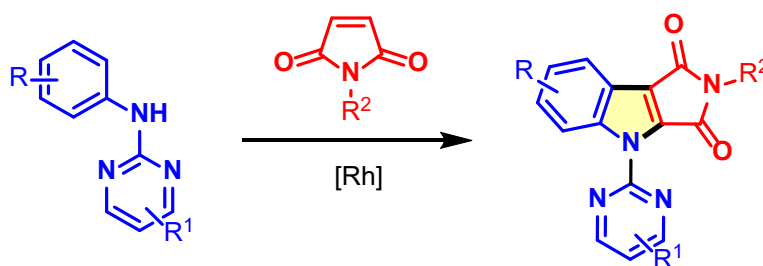
Cyclobutane scaffolds are gaining traction in medicinal chemistry because their rigidity locks substituent vectors in space, enabling tighter control over bioactive conformations. Adding fluoroalkyl groups to these strained rings further broadens their physicochemical space, making them appealing building 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).

Rh(III)-Catalyzed [3+2] Annulation via C(sp²)-H Activation for the synthesis of pyrimidinyl-embedded pyrrolo[3,4-*b*]indoledionesYong Rok Lee^{1*}, Muhammad Saeed Akhtar¹, Mohammad Aslam¹, Sonaimuthu Mohandoss¹¹School 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).

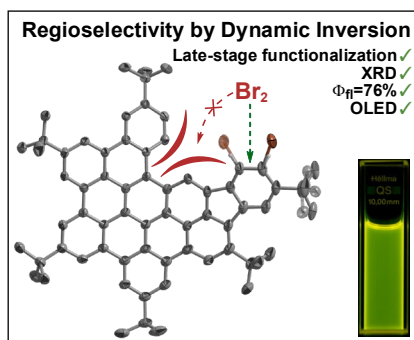
OLED material by late-stage functionalization of hexa-*peri*-benzocoronene-fluoranthene hybrid directed by dynamic inversion of helicity

Lina M. Filla^{1,†}, Alexander R. Krappe^{1,†}, Jacob C. Mayer², Jan M. Sühlo³, Larissa S. Eitelhuber¹, Anja Wiesner¹, Lukasz Polewski¹, Ute Resch-Genger⁴, Beate Paulus¹, Emil J. W. List-Kratochvil³, Siegfried Eigler^{*1}

¹Freie Universität Berlin, Germany; ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany;

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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·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.



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MDR - D1 - P10

Enhancing organic electrochemical transistor performance through synthesis of polythiophene with carbonyl ester-bridge ethylene glycol side chains and investigating extended conjugation effects

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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.

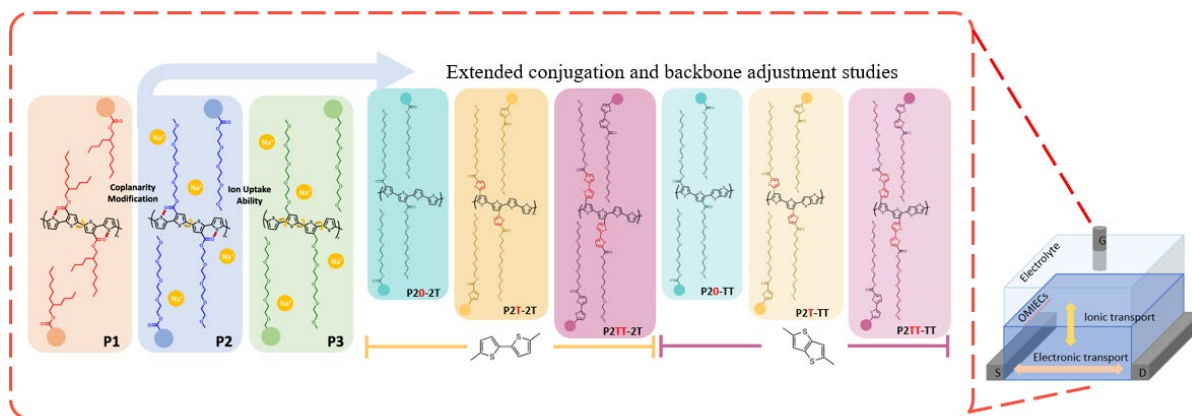


Fig. 1. Overview of side-chain engineering and backbone conjugation strategies in polythiophene-based conjugated polymers for OECT applications. The design integrates PEG side-chain modification, alkyl spacing, and backbone conjugation extension to systematically explore their roles in regulating mixed ion–electron transport.

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¹University 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; ³University of Bucharest, Faculty of Chemistry, Dept. of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Romania; ⁴University of Bucharest, Faculty of Interdisciplinary Studies, Dept. of Interdisciplinary Studies, Romania

***N*-acylhydrazones**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 compounds², synthesis of 2,5-disubstituted-1,3,4-oxadiazoles³, photoswitching molecules⁴, macrocycles⁵, dynamic polymers (dynamers)⁶ or covalent organic frameworks⁷. We have recently described synthesis of novel [2 + 2] and [3 + 3] ***N*-acylhydrazone**-based macrocycles⁸ 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

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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 spatiotemporal control of biological systems². 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 coordination⁴. 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

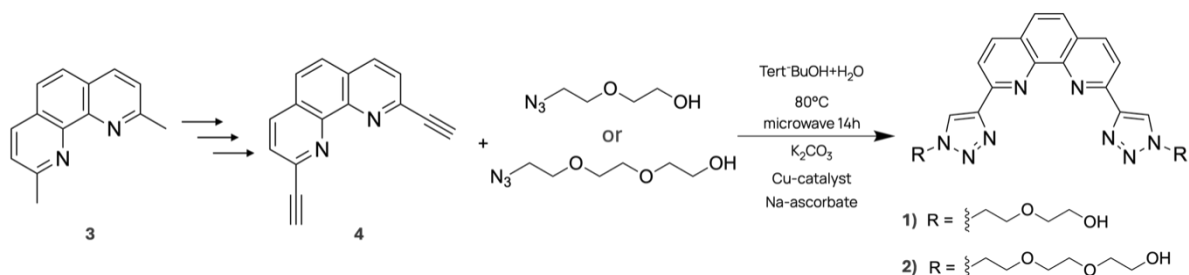
Innovative hydrophilic ligands for the selective recovery of Am(III) from spent nuclear fuel

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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 properties¹. 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 (²⁴¹Am, ²⁴⁴Cm, and ¹⁵²Eu) 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 SO₃-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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Single-molecule force spectroscopy of a trefoil knot gated by a Diels-Alder mechanophore

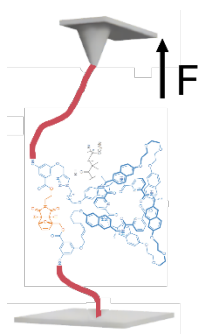
Martin Blavier¹, Min Zhang^{2,3}, Robert Nixon², Guillaume De Bo², David A. Leigh^{2,3}, Anne-Sophie Duwez¹¹University of Liège, Belgium; ²University of Manchester, United Kingdom; ³East China Normal University, China

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 material², as can be revealed experimentally using single-molecule techniques³. 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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A diastereoselective synthesis of small $\alpha\alpha$ calix[4]pyrrole building blocks

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Two-walled $\alpha\alpha$ 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 $\alpha\alpha$ /ab calix[4]pyrrole diastereomers and subsequent separation of the diastereomers.² Since most applications only use the $\alpha\alpha$ diastereomer, the $\alpha\beta$ 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 $\alpha\alpha$ 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 $\alpha\alpha$ calix[4]pyrrole building blocks on a synthetically useful scale, we developed a diastereoselective synthesis. Method-optimization led to high yields of $\alpha\alpha$ calix[4]pyrroles. The versatility of the synthesis was demonstrated by the preparation of different targets. Further, methods for chemoselective post-functionalization of those $\alpha\alpha$ 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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³Schmitt, C.; Wasternack, J.; Braune, F.; Müller, S.; Fasting, C.; Bombei, D.; Eigler, S.; Schalley, C. A., unpublished work.

MDR - D1 - P16

A scalable and resource-saving synthesis of dipyrromethanes and tetrapyrroles - minimal polymer formation and facile purification^{1,2}

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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.



¹Wasternack, J.; Schrit, C.; Steiner, L.; Specht, O.; Braune, O.; Balizs, M.; Müller, S.; Wiesner, A.; Paulus, B.; Eigler, S.; Schalley, C. A. *Adv. Synth. Catal.*, accepted Dec **2025**.

²Wasternack, J.; Schrit, C.; Specht, O.; Schalley, C. A.; Müller, S., Synthesis method for obtaining dipyrromethanes and tetrapyrroles [Unpublished work, patent filed]. Institut für Chemie und Biochemie, Freie Universität Berlin, July 29, **2025**.

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MDR - D1 - P17

Bicyclic 1,4-dioxepanes - novel advanced building blocks for drug discovery

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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).

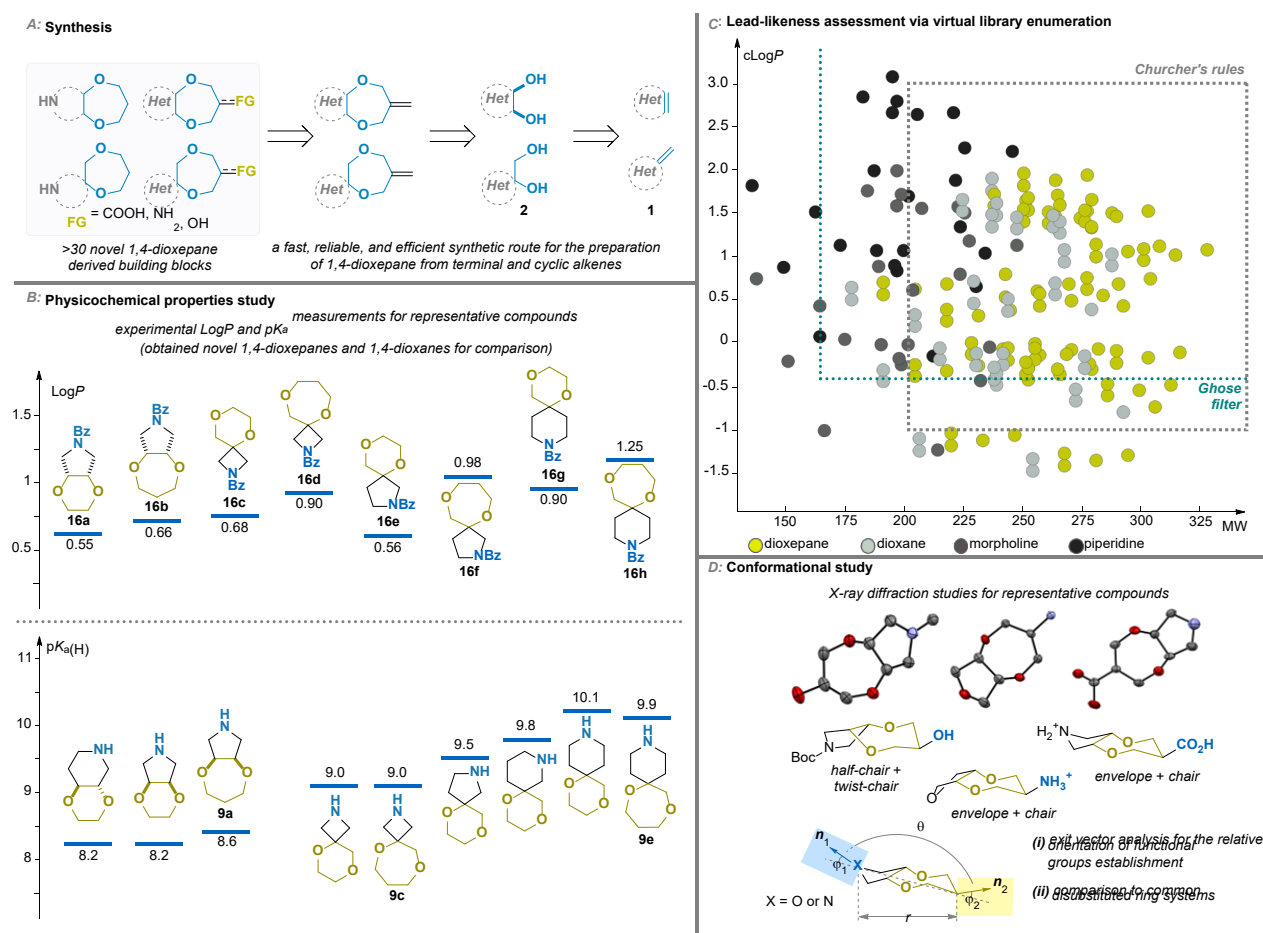


Fig. 1. (A) Retrosynthetic approach to the target saturated bicyclic 1,4-dioxepanes. (B) ORTEP diagrams and conformations of compounds. (C) p*K*_a(H) and Log*P* values for compounds. (D) MW – cLog*P* plot of the generated virtual library.

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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 SO₂ 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.

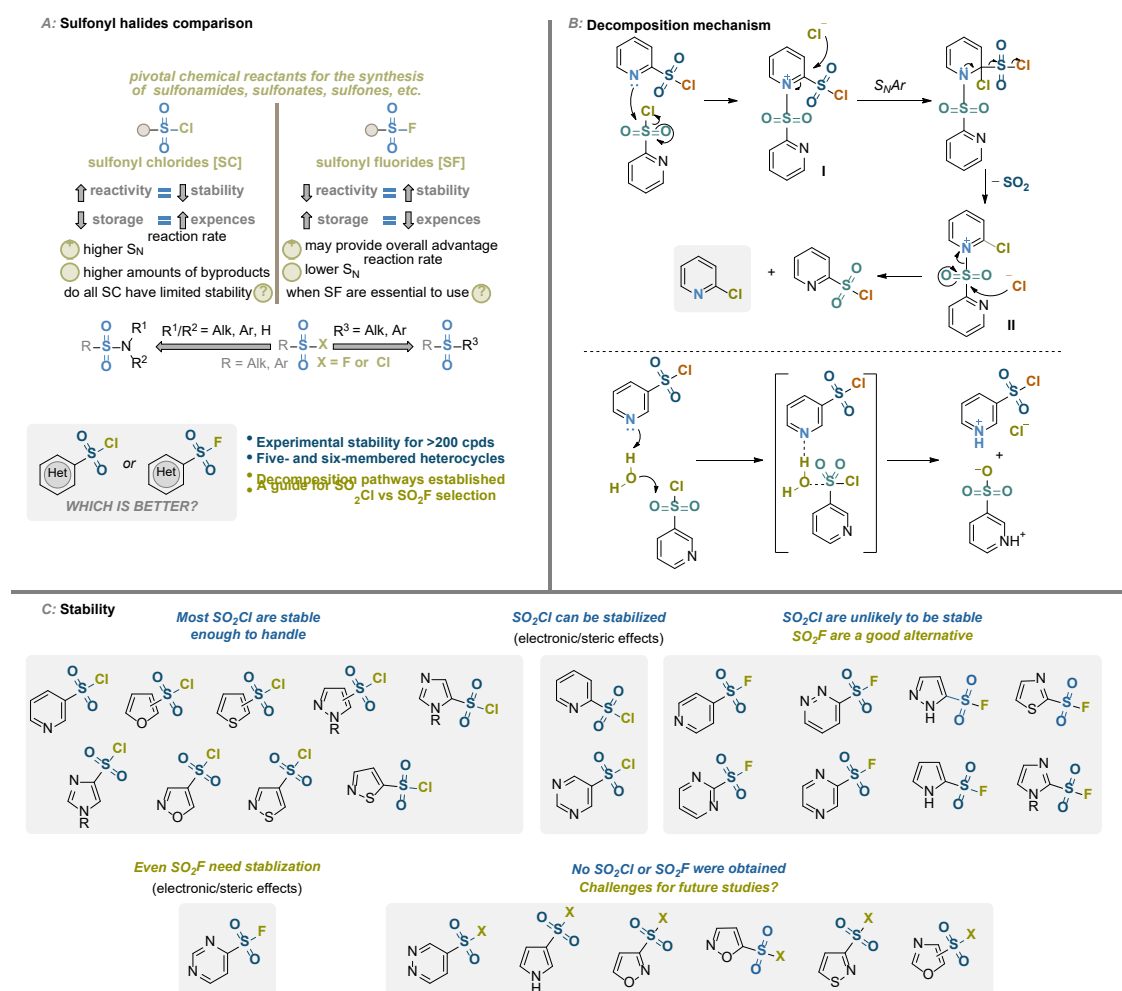


Fig. 1. (A) Sulfonyl chlorides versus sulfonyl fluorides. (B) A proposed mechanism for the decomposition of sulfonyl chloride compounds. (C) Stability guidelines for heterocyclic sulfonyl halides (chlorides vs fluorides).

Letícia D. Costa^{1,*}, Nuno M. Moura¹, Amparo F. Faustino¹, Augusto C. Tomé¹¹LAQV-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 Cu²⁺ (**Figure 1**) will be also discussed.

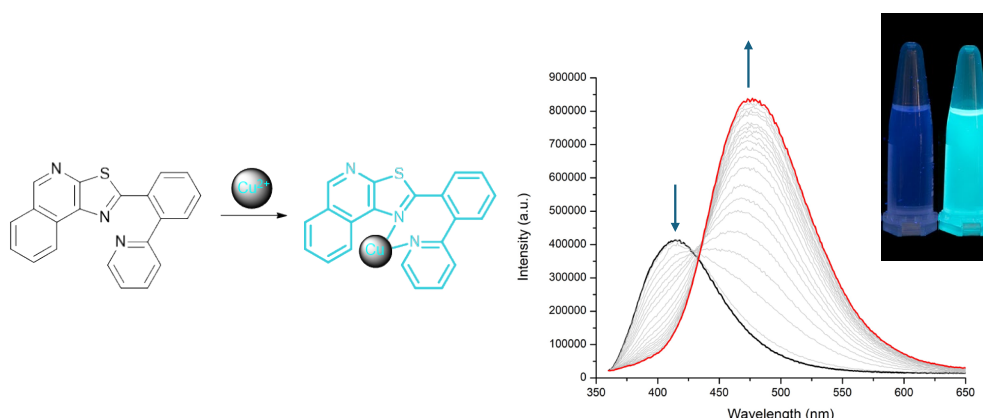


Fig. 1. Increased fluorescence emission of TzIQ in the presence of Cu²⁺.

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

Difluoromethoxy group as a new MedChem handle

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¹Enamine Ltd, Ukraine; ²Institute of Organic Chemistry, Ukraine; ³Taras Shevchenko National University of Kyiv, Ukraine; ⁴Enamine Scientific Research Institute, Ukraine

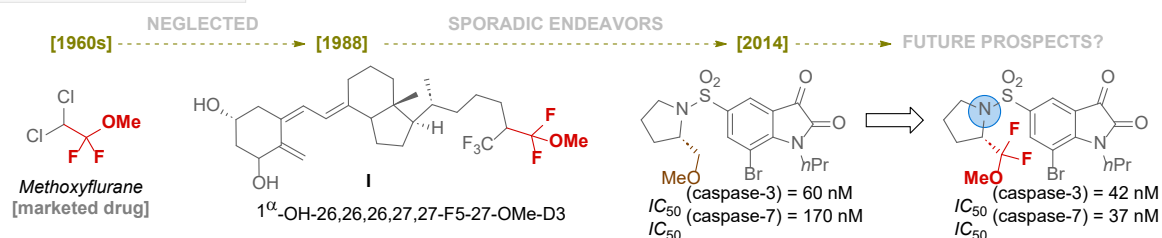
Fluorination has become a routine strategy for modulating potency, selectivity, and ADMET properties in contemporary medicinal chemistry. As the field gradually shifts from aromatic fluorination toward more three-dimensional and metabolically robust aliphatic motifs, access to unconventional fluorinated fragments becomes a defining bottleneck. One of the most promising, yet curiously underexplored, substituents is the difluoro(methoxy)methyl (CF₂OMe) 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 CF₂OMe from an “interesting idea” into a routine MedChem handle. We developed a modular, operationally straightforward platform for preparing CF₂OMe-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.

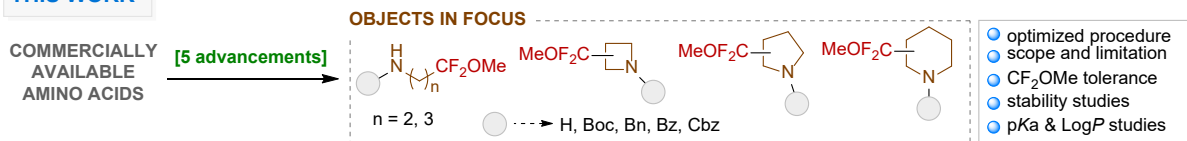
A central enabling element is an imidate-based thionation strategy that delivers diverse thionoesters from both cyclic and acyclic amines, thereby establishing a scalable entry to the fluorination step. Systematic reaction mapping revealed structure-dependent performance trends and practical constraints (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 CF₂OMe 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 CF₂OMe 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 CF₂OMe further support its attractiveness for MedChem and agrochemical applications.

MedChem background



THIS WORK



¹Pashko, M.; Granat, D.; Leha, D.; Yagupolskii, Y.; Volochnyuk, D.; Ryabukhin, S. *ChemRxiv*. 2025; doi: 10.26434/chemrxiv-2025-1k503.

MDR - D1 - P21

Synthesis and characterization of the silver (I) tranexamate complex with potential antibacterial activity

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¹Farmacia 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.

7.1. ANÁLISIS DE ESPECTROFOTOMETRÍA INFRARROJA FTIR DE TRANEXAMATO DE PLATA

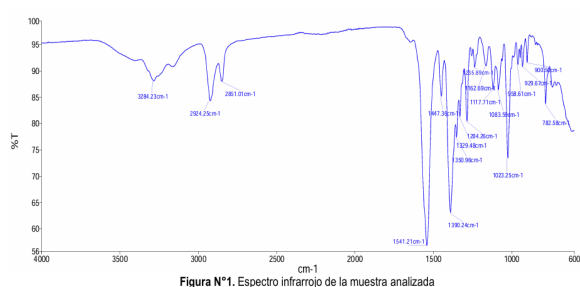


Figura N°1. Espectro infrarrojo de la muestra analizada

Fig.1. FTIR Analysis of Silver Tranexamate

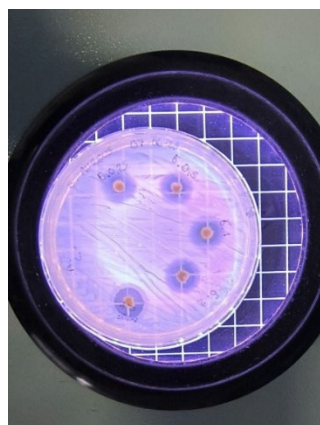


Fig. 2. Antibacterial Activity against *Staphylococcus aureus*

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

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¹VSB - Technical University of Ostrava, Czech Republic; ²CSIR-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.

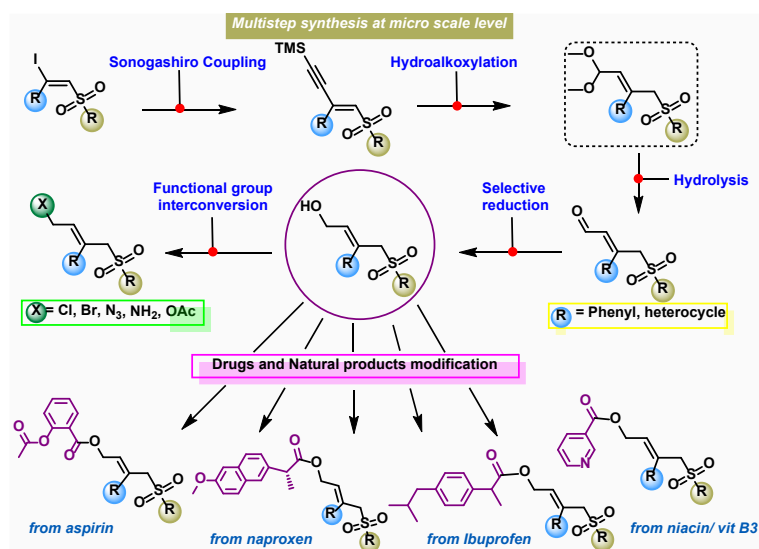


Fig. 1. Synthesis of Diverse Allylic Sulfone Derivatives.

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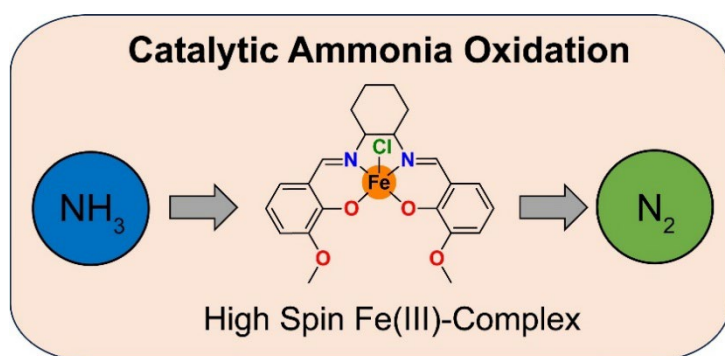
¹Zeng, J.-H.; Li, D.-C.; Zhang, S.; Zhan, Z.-P. *Org. Lett.* **2022**, *24*, 1195–1200.

²Xie, P.; Sun, Z.; Li, S.; Cai, X.; Qiu, J.; Fu, W.; Gao, C.; Wu, S.; Yang, X.; Loh, T.-P. *Org. Lett.* **2020**, *22*, 4893–4897.

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Catalytic ammonia oxidation mediated by high-spin Fe(III) complex: Combined experimental and DFT studyMohammad Usman¹, 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 Fe(III)-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 triarylammonium 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.

¹Usman, M.; Hussein, M. AT.; Kandiel, T. A.; Yamani, Z. H.; Shaikh, M.N. *Catal. Sci. Technol.*, **2026**, 16, 124-136.² Zott, M. D.; Garrido-Barros P.; Peters, J. C. *ACS Catal.*, **2019**, 9, 10101–10108.³Zott, M. D.; Peters, J. C. *J. Am. Chem. Soc.*, **2021**, 143, 7612–7616.