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Perspectives in Analytical & Physical Chemistry (APC)

APC - D3 - P01

Determination of dopant elements in optical crystals with solid sampling high-resolution continuum source graphite furnace atomic absorption spectrometry

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High-purity lithium niobate ($LiNbO_3$) crystals are attractive hosts for nonlinear optical applications, and therefore, are the subject of extensive physical−chemical studies. These crystals are usually grown from melts of metal oxides using Czochralski or high-temperature top-seeded solution growth (HTTSG) methods. The optical properties of the crystal can be tuned with specific dopants added as oxides to the starting materials before crystal growth. Bismuth is an outstanding dopant, exhibiting real-time holographic display and long-lived photochromic signals in lithium niobate. Potassium is used in an oxide form during growth as a flux material, therefore it can be incorporated into the crystal host's lattice and negatively influences the physical-chemical properties.

In this study, methods were developed for the characterization of these dopants, using high resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS-GFAAS) with solid sampling. Samples were dispensed into graphite boats and weighed on a microbalance. Conditions were optimized by varying the parameters of the graphite furnace heating program and dispensing different masses of the pulverized crystal samples into the graphite boats.

Analytical lines of Bi I 227.658 nm and K I 404.414 nm were selected for the method. In solid sampling GFAAS, calibration is a challenging task, due to the lack of solid standards of matching and well-known elemental composition. Consequently, standard solutions were applied for calibration, based on the standard addition method for the solid sample. For this purpose, two means of calibration were utilized, i.e., common standard addition and the three-point estimation standard addition (Fig. 1). The analytical results obtained with both calibration methods showed good agreement. The LODs were found to be 0.32 and 0.53 µmol/mol, respectively. The Bi and K content of the crystal samples were in the range of 3.9-19.4 µmol/mol and 0.45-1.12 µmol/mol, respectively. The accuracy of the methods was verified against solution introduction HR-CS-GFAAS.

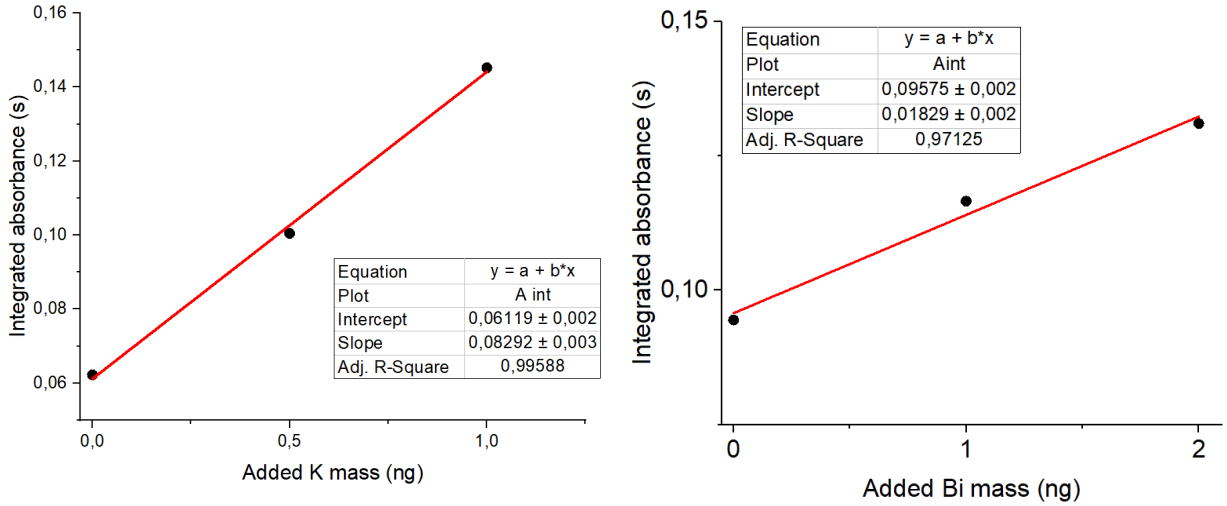

Fig. 1. Three-point estimation standard addition calibration of Bi and K in a lithium niobate sample

APC - D3 - P02

Studies on the improvement of the electrolyte cathode atmospheric glow discharge for environmental monitoring purposes

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Electrolyte cathode atmospheric glow discharge (ELCAD) is a DC microplasma, which was developed for optical emission spectrometry (OES) monitoring of environmental samples.[1] A common example of their application is the on-line monitoring of metal contaminants (e.g., Cd, Cu, Ni, Pb, Zn) in natural and wastewaters.[2] In principle, the ELCAD technique utilizes the direct introduction of certain aqueous solution (electrolyte) samples without the need for any additional sample dispersion unit (e.g., nebulizer), common in atomic spectroscopy techniques (e.g., inductively coupled plasma OES, flame AAS/OES). However, this simplicity and the small plasma volume of ELCAD is a drawback, which gives rise to various spectral and non-spectral interferences.[3] For instance, due to the direct introduction of aqueous solutions, the plasma is saturated with water vapour and related plasma species (e.g., OH-radicals), which cause the appearance of intensive OH-bands in the emission spectra (Fig. 1).
In this work, some novel findings of the ELCAD-related research are presented, e.g., the use of alternative atmospheres (e.g., Ar) around the glow discharge, chemically modified aqueous media for the standard/sample electrolytes to counteract interference effects and/or to enhance the emission intensities of analytes. The optimization of the conditions (sample solution pH, sample flow rate, plasma observation height, anode–cathode distance, etc.) will be discussed. The results will be compared in connection with regular solution media applied in ELCAD and alike plasma spectroscopy methods. The analytical results will be highlighted through some examples of direct sample analysis, including natural waters.

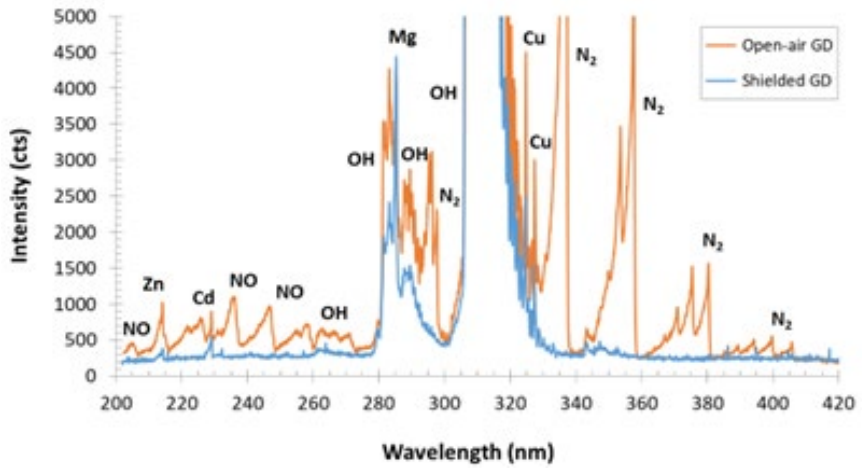

Fig. 1. Spectra of ELCAD recorded with an open-air and a shielded GD-cell (50 ppm Cd, Cu, Zn, Mg in HCl, pH 1.53).

APC - D3 - P03

Artificial intelligence-assisted optimization of an HPLC method for the determination of levetiracetam and piracetam

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Levetiracetam (LEV) is a modern antiepileptic drug with broad clinical application in seizure management. Piracetam (PIR) is a neuroactive nootropic agent that enhances cognitive performance and is frequently used in neurological therapies[1-6]. Accurate analytical monitoring of these compounds requires robust and optimized chromatographic methods. In recent years, studies integrating artificial intelligence with HPLC methodologies have increasingly emerged[7]. This study presents an artificial intelligence (AI)-assisted approach to the development of a high-performance liquid chromatography (HPLC) method for the simultaneous determination of LEV and PIR. Chromatographic parameters, including mobile phase composition, flow rate, and temperature, were experimentally varied to generate a dataset representing analytical system behavior. Machine learning models were trained using experimental chromatographic data to describe nonlinear relationships between operational parameters and analytical responses such as retention time, resolution, and analysis duration. The trained models were employed as predictive tools to estimate analytical performance under untested experimental conditions. The AI system enabled multi-objective optimization by simultaneously considering chromatographic separation efficiency and operational performance. Using this predictive framework, optimal chromatographic conditions were obtained with fewer experimental trials, reducing experimental workload and resource consumption. The predicted optimal conditions were experimentally verified, demonstrating good agreement with model predictions. The study demonstrates that artificial intelligence can function as a decision-support tool in chromatographic method development rather than replacing experimental validation. Integrating data-driven modeling with laboratory experimentation allows rational optimization of analytical methods and improves efficiency. The proposed workflow indicates that combining chromatography and artificial intelligence provides a promising strategy for modern analytical chemistry, offering faster method development, reduced trial-and-error experimentation, and improved analytical reliability.

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APC - D3 - P04

LC-MS/MS method development and validation for clinical pharmacokinetics and therapeutic drug monitoring of potassium-competitive acid blocker vonoprazan-based triple therapy for H. pylori in human plasma

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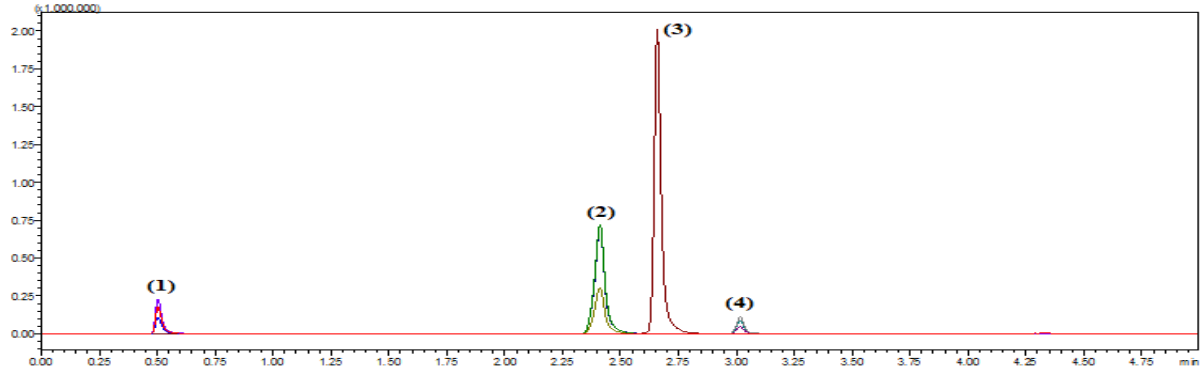
A newly FDA-approved triple therapy for Helicobacter pylori eradication combines vonoprazan (VPN), a potassium-competitive acid blocker, with amoxicillin (AMX) and clarithromycin (CMN). This study reports the development and full validation of a rapid, selective, and sensitive LC-MS/MS method for simultaneous quantification of these drugs in spiked human plasma. Sample preparation employed a straightforward liquid–liquid extraction (LLE) procedure. Chromatographic separation was completed within 5 minutes using a Phenomenex Kinetex C18 column (100 × 4.6 mm, 2.6 µm) with a gradient elution of 0.1% formic acid in water and acetonitrile. Diazepam served as an internal standard, and mass spectrometric detection was performed in multiple reaction monitoring (MRM) mode with positive electrospray ionization. The method demonstrated excellent linearity across the tested ranges (2–100 ng/mL for AMX and CMN; 5–100 ng/mL for VPN). Both intra- and inter-day precision and accuracy complied with FDA bioanalytical validation guidelines, with relative standard deviations and errors below 15%. Mean absolute recoveries exceeded 93% for all analytes. Greenness assessment using the AGREE tool confirmed the method's environmental friendliness. Overall, the validated LC-MS/MS method provides a rapid, reliable, and eco-friendly approach for simultaneous determination of VPN, AMX, and CMN in human plasma, supporting its potential application in clinical pharmacokinetic and therapeutic monitoring studies.



Total ion chromatogram (TIC) chromatograms for Amoxicillin (1), Vonoprazan Fumarate (2), Clarithromycin (3), and Diazepam (4) at 10 ng/mL.

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APC - D3 - P05

Forensic characterization of cannabis in vape products and labeled products seized in two court cases: A case study

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The rapid emergence of electronic cigarettes containing cannabis-derived constituents presents significant analytical and interpretative challenges for forensic laboratories. Illicit vape products incorporating psychoactive substances like Δ^9-tetrahydrocannabinol (THC), cannabidiol (CBD), and cannabinol (CBN) from *Cannabis sativa L.* pose growing public health and regulatory concerns. This necessitates robust analytical workflows for their accurate identification in seized materials.

Case Report including Results: This report details the forensic examination of two court productions submitted to Sri Lanka's Government Analyst's Dept., which included vape products and labeled joint materials. A systematic analytical workflow was employed, comprising visual examination, presumptive testing with Fast Blue B reagent, and thin-layer chromatography (TLC) for screening, followed by conclusive gas chromatography–mass spectrometry (GC–MS) for definitive confirmation.

Visual inspection revealed brown, viscous liquids within the vape devices and dried herbal material in the joints. Presumptive testing with Fast Blue B yielded a characteristic red coloration, indicating phenolic cannabinoids, while TLC analysis showed results consistent with cannabinoid reference standards. The definitive GC–MS analysis confirmed the presence of Δ^9-THC, CBD, and CBN in all samples. Furthermore, a terpene profile rich in limonene, linalool, β-caryophyllene, and α-humulene supported a natural cannabis origin. The detection of glycerol triacetate (triacetin), a common e-liquid additive, exclusively in the vape liquids confirmed their deliberate formulation for vaping.

Conclusion: The combined analytical approach provided definitive forensic evidence of natural cannabis constituents in both vape liquids and joint materials. These findings highlight an emerging forensic and regulatory challenge, underscoring the critical need for enhanced monitoring and analytical preparedness in forensic laboratories to address the proliferation of these products, thereby ensuring public safety and supporting regulatory enforcement.

Keywords: Vape products; Δ^9-THC; cannabinoids; GC–MS.

APC - D3 - P06
Silver nanoparticle synthesis using a deep eutectic solvent and green tea

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There are environmental and health hazards associated with conventional organic solvents used in metal nanoparticle (MNP) synthesis; Deep Eutectic Solvents (DESs) are a sustainable alternative and an appealing medium for green chemistry. In traditional MNP synthesis, toxic stabilizers such as cetyltrimethylammonium bromide, sodium dodecyl sulfate, and polyvinylpyrrolidone are used to provide electrostatic or steric repulsion.[1] However, DESs can play multiple active roles in MNP synthesis, simplifying the process and reducing the need for additional reagents.

This research employed a DES composed of betaine and glycerol (1:3) first to extract natural compounds from green tea and then to synthesize silver nanoparticles (AgNPs) using the extracted tea and silver sulfate. The tea extract was analyzed using UPLC-UV to quantify caffeine and gallic acid, both crucial in AgNP synthesis. MNP optical properties were characterized using UV-Vis spectroscopy, and the hydrodynamic diameter in aqueous suspension was measured by DLS. The size and morphology of the AgNPs were examined by TEM, while synthesis efficiency was determined by ICP-MS.

UPLC analysis allowed optimization of the extraction conditions of 90 °C and 75 minutes. The AgNPs synthesis using the DES-assisted green tea extract was optimized and the resultant particles were comprehensively evaluated. The effect of country of origin of green tea on the AgNP synthesis was investigated. AgNPs synthesized from Aldi green tea leaves under optimized conditions revealed a λ_{max} at 432 nm (**Figure 1A**), with a mean particle size of 19.6 nm (**Figure 1B**) measured by UV-Vis spectroscopy and TEM, respectively.

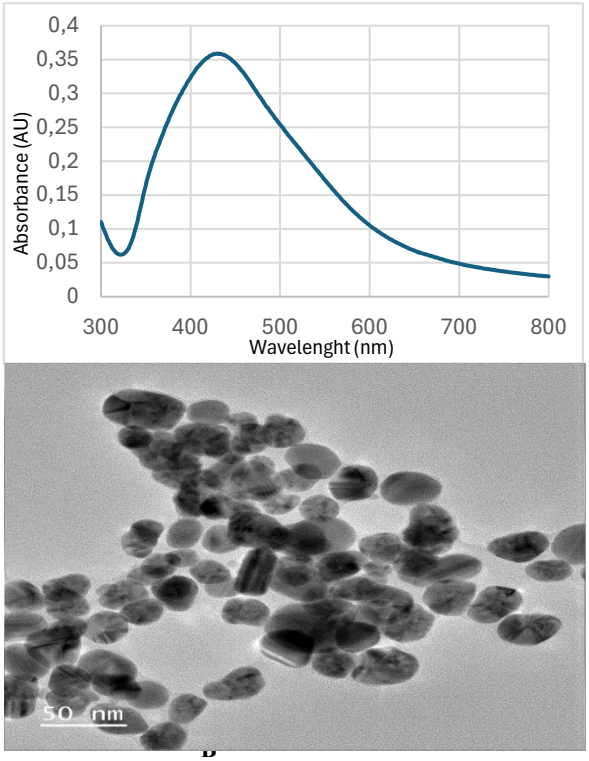

Fig. 1. (A) UV-Vis spectrum and **(B)** TEM image of AgNPs synthesized using 1 mL of extracted Aldi green tea, 3 mL of Bet:Gly (1:3) DES, and 0.025 g of silver sulfate at 90 °C for 75 minutes under stirring.

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APC - D3 - P07

Green twist to solvent extraction and separation of metallic species with elfin chelating ligands

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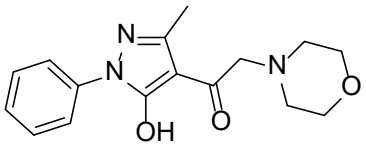
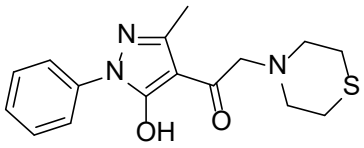
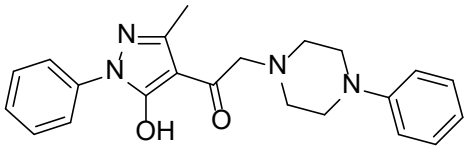
The competitive solvent extraction of various metal species in the periodic table by a series of ligands, tested for the first time, composed of N-heterocyclic receptors with variable ring size and one β-dicarbonyl fragment have been conducted to get a snapshot of their efficacy. The effect of heteroatoms in the substituent on the extraction performance and selectivity of this type of chelating extractants with equivalent binding sites but an unsymmetric backbone due to differing coordination environments has been evaluated. The effect of chemical nature of the organic liquid phase on the extraction process was also discussed: ionic liquids (IL, $[C_1C_nim^+][Tf_2N^-]$) or typical organic diluents. The superiority of the IL medium has been demonstrated. Nevertheless, the coordination capacity of the chelating agents is somehow meticulously dependent on the oxidation state of the extracted chemical element. The extraction capacity and selectivity of ligands towards lanthanoids were found to decrease on going from HL6 and HLO to $HLNC_6H_5$ and HLS. Generally, the decrease of extraction efficiency for compound HLS in comparison with other investigated molecules in an IL medium could be attributed to its solubility characteristics because in chloroform this ligand shows better extraction properties than others. The separation factors between adjacent metals of 4f-series and iron towards other metal ions have been assessed. Furthermore, EPR, Raman and DTA-TG-MS spectroscopies have been used to study the extracted d- and f-chelate complexes in the obtained extracts in IL solutions: Gd^{3+} and Fe^{3+}.



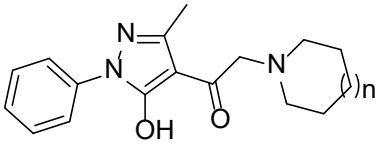
HLO



HLS



$HLNC_6H_5$



HL5 - n=0
HL6 - n=1
HL7 - n=2
HL8 - n=3

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APC - D3 - P08
Drug release performance of amphiphilic polymeric micelles and cross-linked micelles

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Micellar systems formed through the self-assembly of amphiphilic polymers have attracted significant attention due to their remarkable potential in drug delivery applications. Although polymeric micelles offer several advantages, including enhanced solubility of hydrophobic drugs, controlled release behavior, and biocompatibility, their structural instability under varying pH, temperature, or concentration conditions remains a major limitation. To overcome these challenges, chemical modification and cross-linking strategies have been widely employed to improve micellar stability and performance under physiological conditions. Accordingly, numerous studies in the literature have focused on the design and application of cross-linked amphiphilic polymeric micelles as robust and efficient carriers for drug delivery systems [1–3].
In the present study, a triblock copolymer, poly[(ethylene glycol) methyl ether methacrylate]-*b*-poly[(2-(dimethylamino)ethyl methacrylate]-*b*-poly[(2-(diisopropylamino)ethyl methacrylate] (PEGMEMA-*b*-PDMA-*b*-PDPA), was successfully synthesized. The amphiphilic copolymer was characterized by proton nuclear magnetic resonance spectroscopy and gel permeation chromatography. Micellar solutions were obtained by adjusting the pH of the block copolymer solution, while cross-linked micelles were prepared through the cross-linking of the inner PDMA-corona. The hydrodynamic diameters of the micelles and cross-linked micelles were determined using dynamic light scattering. The *in vitro* release behavior of the model drug dipyridamole was evaluated in phosphate buffer solution at pH 7.4. The results demonstrated that both noncross-linked and cross-linked micellar systems exhibit favorable characteristics, highlighting their potential applicability as effective drug delivery platforms.

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APC - D3 - P09

Influence of silane-based monolayers on the stability and transformation of β-glycine using SHG microscopy

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Controlling nucleation and polymorphic outcomes remains a key challenge in pharmaceutical crystallization. Various polymorphs of the same compound can exhibit distinct solubility, stability and bioavailability, so preventing unwanted polymorphic transition is crucial for ensuring drug quality, efficacy and safety[1,2]. Glycine serves as an ideal model for such studies due to its well-characterized polymorphs at ambient conditions (α-glycine, β-glycine and γ-glycine). It is well known that the least stable β-glycine can be formed under kinetically controlled conditions (e.g. at low supersaturation, antisolvent addition or confined crystallization)[3–6]. However, this polymorph is particularly difficult to isolate, as it rapidly converts into the thermodynamically stable α-glycine via solution-mediated transformation[7,8]. Here, we investigate how interfacial chemistry can modulate the kinetic landscape of glycine crystallization using silane-based monolayers bearing different terminal functional groups ($–NH_2$, –pyridyl, –F), alongside hydroxyl rich piranha cleaned substrates. β-glycine was crystallized via evaporative microdroplet confinement with methanol as anti-solvent. Second Harmonic Generation (SHG) microscopy was used for real-time, spatially resolved monitoring of polymorphic distribution and transformation. As a symmetry-sensitive technique, SHG provides intrinsic contrast between the non-centrosymmetric SHG active β form ($P2_1$) and the centrosymmetric SHG-silent α form ($P2_1/n$), allowing direct visualization of phase transformation kinetics at the solid-liquid interface[9].

Our findings reveal that crystal size distribution and the stability of β-glycine strongly depend on the surface chemistry of the functionalized substrate. Hydrophilic surfaces capable of forming strong hydrogen bonding ($–NH_2$ and –OH) extended the lifetime of β-glycine, likely through stabilizing its polar crystals faces and raising the energetic barrier for solution-mediated transformation, in contrast to rapid conversion on a hydrophobic fluorinated surface. Furthermore, 3D SHG imaging revealed spatial heterogeneity with SHG active β domains and SHG inactive α domains coexisting in individual crystals. Polarization-resolved SHG microscopy was also performed on selected SHG active crystals to gain deeper insight into crystal symmetry and molecular orientation. By combining P-SHG with 3D SHG imaging, polymorphic distribution and transformation pathways could be directly correlated with interfacial chemistry.

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APC - D3 - P10

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

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

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

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

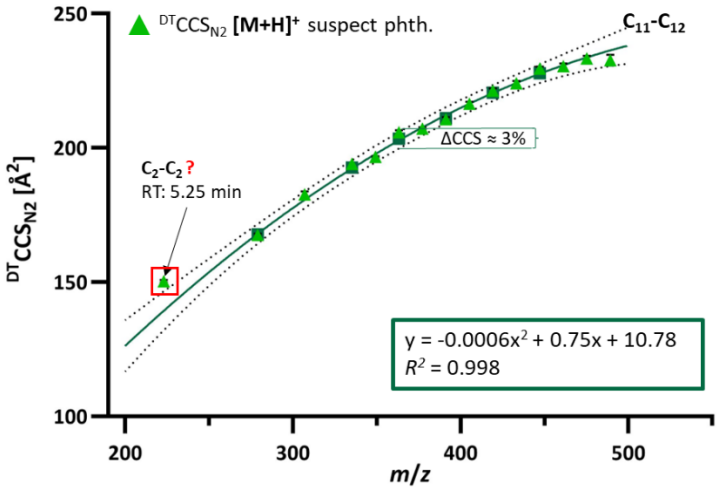

Fig. 1. CCS-*m*/*z* trendline describing the relationship between collision cross section (CCS) value and mass-to-charge (*m*/*z*) ratio. Dark-green squares represent CCS values calculated from phthalate reference standards. The corresponding CCS-*m*/*z* trendline was fitted using a 2nd order polynomial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

APC - D3 - P11
Synthesis and crystalline structure of diaquabis (5-methylthiazole-2-carboxylate-κ2N,O) cobalt (II)

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Institute of Bioorganic Chemistry Academy of Sciences of the Republic of Uzbekistan

Cobalt (II) acetate tetrahydrate (0.249 g, 1.0 mmol) was dissolved at room temperature in 2 ml of deionized water until complete dissolution. At the same time, 5-methylthiazole-2-carboxylic acid[1] (0.286 g, 2.0 mmol) was dissolved in 4 ml of absolute ethanol at a temperature of 60°C. The two transparent solutions were gradually combined under constant stirring. The resulting mixture was filtered through a 0.45 μm membrane filter. The filtered solution was left in an open container at room temperature (298 ± 2 K) for slow evaporation. After 10 days, green monocrystals suitable for X-ray analysis were formed. The product was separated by filtration, washed with cold ethanol, and air-dried. The yield (relative to cobalt) was 80%.

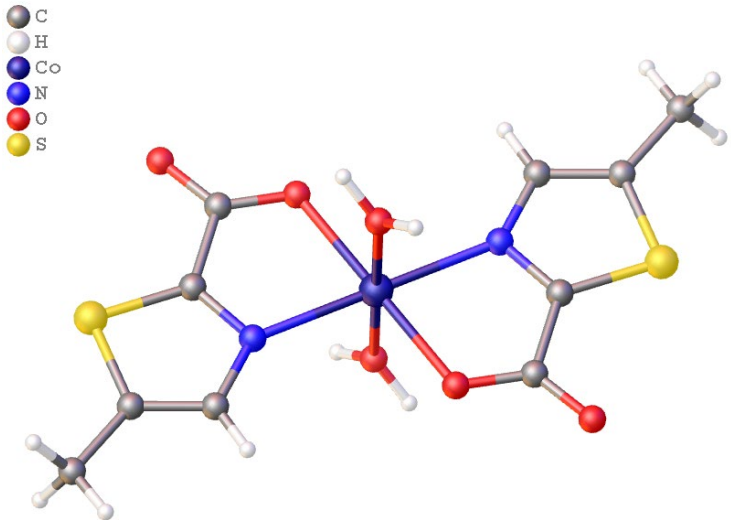

Fig. 1. Molecular structure of diaquabis (5-methylthiazole-2-carboxylate-κ2N,O) cobalt (II)

The substance crystallizes in a monoclinic P21/c space group, with four formula units in the unit cell. The central cobalt (II) ion is located in a slightly distorted octahedral-shaped coordination medium. It is bonded to two nitrogen atoms (Co-N 2.126 (6) Å) and four oxygen atoms of two 5-methylthiazol-2-carboxylate ligands: two from monodentate carboxylate groups (Co-O 2.133 (5) Å) and two from bound water molecules (Co-O 2.062 (4) Å). The carboxylate groups are monodentately coordinated, and the thiazole rings are located almost in the same plane as the coordination plane.
The crystal structure was determined using Cu Kα radiation at a temperature of 293 (2) K. The data were collected on an Xcalibur Ruby diffractometer[2]. The structure was solved by the charge flipping method and refined to the values of R1 = 0.1029 (I ≥ 2σ (I)) and wR2 = 0.2800 (all data).
Gratitude This study Uzbekistan. Supported by research grant number FL-9524115091 of the Institute of Bioorganic Chemistry of the Academy of Sciences.

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APC - D3 - P12

Comprehensive analytical evaluation and risk assessment of elastomeric container closure systems for biologics and small molecule parenteral drugs

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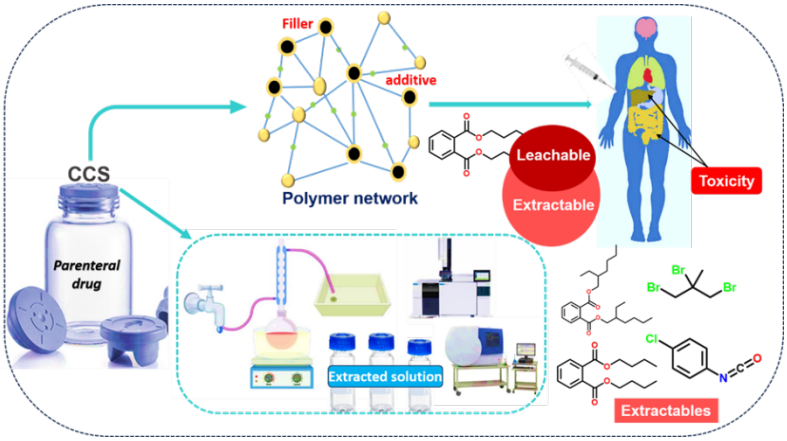
Despite of assuming the chemical inertness of container closure system, bromobutyl stoppers can release extractable and leachable into the formulation that poses significant toxicological risk to human health and it is more concern with the parenteral drugs which bypass first pass metabolism. There is no standardized analytical platform for comparative evaluation of varying stopper size, composition, and surface engineering. This study aims to evaluate the extractables and leachable from different commercially available bromobutyl based rubber stopper by a systematic, orthogonal analytical methods like GC-orbitrap/MS, ICP-AES and 1H NMR to represent the worst-case scenario. Extraction was performed in aqueous solvents at pH 2.5 and 9.5, and in hexane, following USP ⟨1663⟩ and ⟨1664⟩ guidelines. A safety-based Analytical Evaluation Threshold (AET) was calculated for each stopper type, and real-world leachable migration was assessed in two model parenteral drug products biphasic insulin and 2% xylocaine under accelerated aging conditions simulating full shelf-life exposure.

A total of 17, 45, 9, and 18 volatile compounds were identified from RS I–RS IV, respectively, all are below their AET level. Among detected semi volatiles across RS I-RS IV by liquid injection GC-orbitrap/Ms, phthalate esters (dibutyl phthalate, DEHP, DIBP), phenolic antioxidants (2,4-di-tert-butylphenol, BHT), and long-chain hydrocarbons were identified across stopper grades. The most prominent two componenet leached from CCS of biphasic insulin are 2,4-di-tert-butylphenol (up to 12.98 µg/mL) and dibutyl phthalate (up to 7.41 µg/mL) and which are also exceeded respective AET level of 0.935 µg/mL under both accelerated aging condition and normal storage condition. In contrast, aqueous based small molecule drug (xylocaine 2%) leached very less number of compounds. This observation highlighted the role of formulation matrix particularly for biologic samples contains different excipient causes the more leachable migration. Elemental impurities remained below ICH Q3D-based thresholds under all conditions, with the exception of boron in RS I and RS III under acidic extraction. This study demonstrates that stopper composition, size, surface treatment, and extraction pH simultaneously influence the E&L risk profile. The integrated analytical strategy provides a robust framework for chemical characterization and toxicological risk assessment of elastomeric CCS, supporting informed material selection and regulatory decision-making for injectable drugs.

Keywords: Elastomeric container closure system; Extractables and leachables; Parenteral drug safety; GC-Orbitrap MS/MS; ICP-AES; Analytical evaluation threshold.



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Posters

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

CAI - D3- P01

Design, synthesis and biological activity of 2AMINO5,4-B thiazolopyridine EGFR based anti-cancer agent

Mohd Aatif Shaikh
Jamia Hamdard University

The epidermal growth factor receptor (EGFR) plays a central role in tumor development and remains a validated target for anticancer drug discovery. This study demonstrates the integration of computational chemistry and data-driven approaches for the rational design, synthesis, and evaluation of novel 2-amino-5,4-b thiazolopyridine derivatives as potential EGFR-targeted anticancer agents. A library of candidate molecules was rationally designed based on EGFR pharmacophore features and synthesized through a multistep pathway. Structural confirmation was achieved using FT-IR, ^{1}H NMR, and ^{13}C NMR spectroscopy.

Molecular docking simulations were performed against the EGFR tyrosine kinase domain to assess binding affinity and key ligand–receptor interactions. Compounds exhibited favorable docking scores with significant hydrogen bonding and hydrophobic interactions within the ATP-binding pocket, suggesting strong potential for EGFR inhibition. In addition, in silico ADMET and drug-likeness predictions using data-driven tools supported favorable pharmacokinetic properties and compliance with Lipinski's rule of five, indicating drug-like characteristics.

The integration of computational modeling and predictive analytics significantly accelerated lead prioritization and reduced experimental optimization cycles. These results highlight the promising role of computational chemistry and AI-assisted data analysis in guiding the discovery of new EGFR-focused anticancer agents, warranting further biological evaluation.

CAI - D3- P02
From manual operation to autonomous STM via visual reasoning AI

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Scanning Tunnelling Microscopy (STM) is an indispensable tool in surface science and physical chemistry. For instance, this local probe microscopy technique not only allows for the visualization of molecular patterns, monolayer-thin covalent organic frameworks and metal organic frameworks, but also their growth dynamics, with submolecular resolution [1-3]. Yet its operation remains largely manual, time-intensive, and dependent on expert intuition. While many STM systems are built on legacy digital infrastructures, recent access to instrument-level application programming interfaces (APIs) enables new opportunities for advanced automation beyond conventional scripting.

Here, we present a Brain–Puppet hierarchical AI architecture for autonomous STM operation that integrates multimodal visual language models (VLMs) with direct instrument control. A modern external computer hosts a VLM acting as a virtual scientist, which continuously interprets real-time STM images and graphical interface feedback. This enables semantic understanding of experimental states, such as distinguishing molecular features from noise, diagnosing unstable tunnelling conditions, and identifying atomically flat terraces suitable for high-resolution imaging.

High-level experimental strategies generated by the VLM are translated into structured control commands and executed through the STM's native APIs. This hierarchical separation preserves both intelligence and safety, experiment-level reasoning is handled by the AI agent, while the STM's internal feedback loops and PID controllers maintain atomic-scale stability.

By combining visual semantic understanding with instrument-level control, this approach enables adaptive and context-aware experimentation and represents a practical step toward self-driving laboratories in surface chemistry.

Acknowledgements: Financial support from KU Leuven–Internal Funds (C14/23/090), FWO (I006922N), and Chinese Scholarship Council (grant No.202506890042) is acknowledged.

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CAI - D3- P03

Novel antimicrobial agents: From synthetic design to integrated *in vitro* and *in silico* insights

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Antimicrobial resistance (AMR) has emerged as a critical global health challenge driven by the increasing prevalence of multidrug-resistant bacteria, including *Staphylococcus aureus* and *Pseudomonas aeruginosa*, as well as pathogenic fungi such as *Candida albicans* and *C. parapsilosis*. In this study, six newly synthesized Schiff base derivatives (HSB-1 to HSB-6) were systematically evaluated through an integrated experimental and computational approach to identify promising antimicrobial candidates. In vitro antimicrobial screening using disk diffusion assays revealed notable antibacterial activity against *S. aureus*, particularly for HSB-6 and HSB-1 (15–17 mm inhibition zones), while HSB-5 and HSB-6 exhibited measurable activity against *P. aeruginosa* (12 mm). Moderate antifungal effects were observed for HSB-4 against *Candida* species. To rationalize these experimental trends at the molecular level, in silico investigations were performed using molecular docking, molecular dynamics (MD) simulations, density functional theory (DFT), and ADMET profiling. Docking studies demonstrated strong binding affinity of HSB-5 toward the LasR protein of *P. aeruginosa* ($\Delta G = -12.3$ kcal mol^{-1}), supported by favorable hydrogen bonding and hydrophobic interactions. The stability of the protein–ligand complexes was further confirmed by 100 ns MD simulations, showing low RMSD values, compact radius of gyration, and persistent intermolecular interactions. DFT calculations at the B3LYP/6-311G(d,p) level provided electronic descriptors consistent with biological performance, revealing lower HOMO–LUMO energy gaps for HSB-6 and HSB-1 and an intermediate gap for HSB-5. NBO and Fukui analyses identified key electrophilic and nucleophilic sites involved in molecular recognition. ADMET predictions indicated acceptable drug-likeness for most derivatives, including favorable gastrointestinal absorption and physicochemical properties, while highlighting potential safety concerns for selected compounds. Overall, HSB-5 emerged as a balanced lead compound, combining effective in vitro antimicrobial activity with robust computational support, warranting further optimization in the fight against antimicrobial resistance.

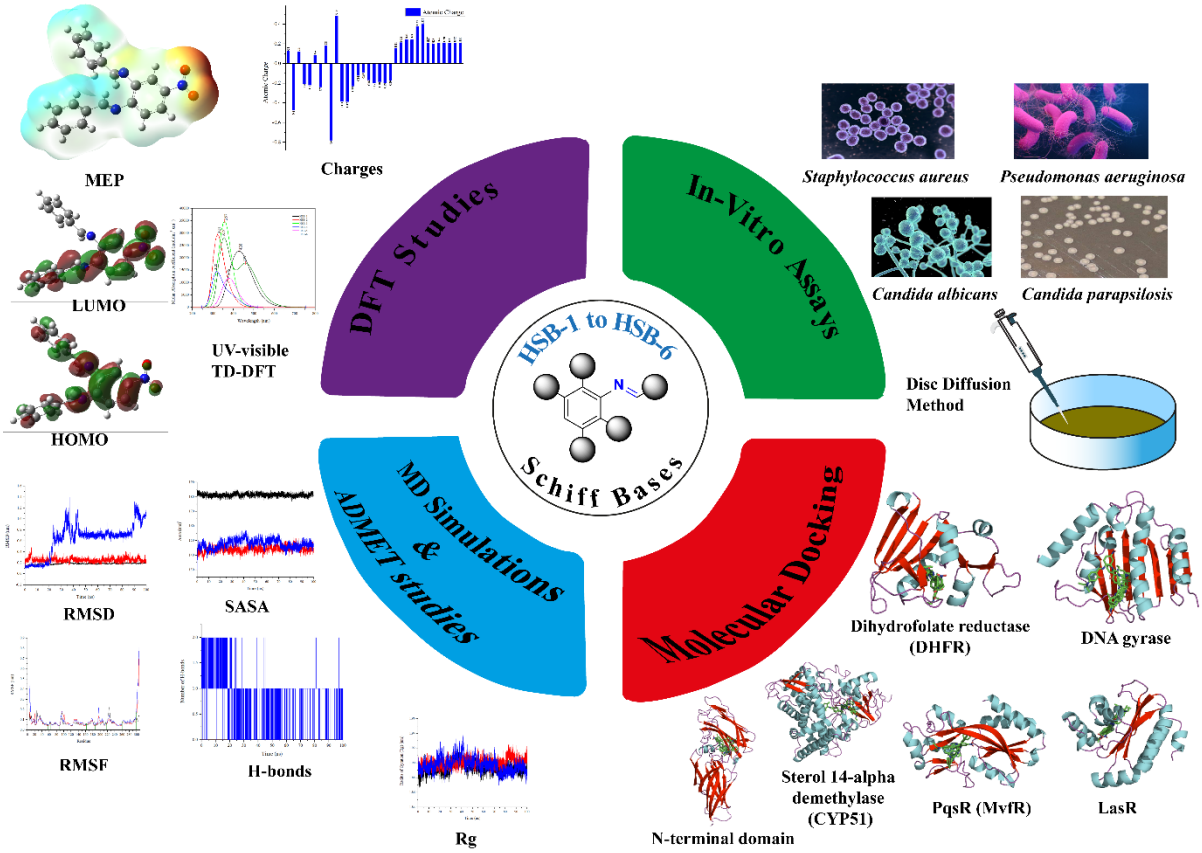

Fig. 1. Diagrammatic illustration of the synthesis of Schiff bases, their antimicrobial activity, and computational evaluation via molecular docking, MD simulations, ADMET, and DFT analysis

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CAI - D3- P04

Data-driven process optimization for selective magnesium recovery from desalination brine

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[1]Interdisciplinary Research Centre for Membrane and Water Security, King Fahd University of Petroleum and Minerals, Saudi Arabia; [2]Dept. of Chemical Engineering, King Fahd University of Petroleum and Minerals, Saudi Arabia; [3]Mechanical Engineering Dept., King Fahd University of Petroleum & Minerals, Saudi Arabia; [4]Dept. of Civil Engineering, Prince Mohammad Bin Fahd University, Saudi Arabia; [5]Dept. of Analytical Chemistry, Faculty of Pharmacy, Near East University, TRNC, Turkey

The sustainable management of desalination brine is increasingly recognized as a critical pathway for both environmental protection and strategic resource recovery. This study presents an integrated experimental–computational framework for the selective recovery of magnesium from real reverse osmosis (RO) reject brine through controlled alkaline precipitation coupled with advanced machine-learning modeling. Magnesium hydroxide ($Mg(OH)_2$) was precipitated using ammonium hydroxide under systematically varied pH (10.0–11.0), temperature (15–35 °C), and initial magnesium concentrations (2100–3148.5 ppm) to delineate the operational recovery window under realistic brine chemistry. Experimental results demonstrate that pH is the dominant governing parameter for magnesium recovery, while temperature exerts a secondary kinetic influence. Under optimized conditions (pH 11, 35 °C, Mg = 3148.5 ppm), magnesium recovery reached 96.91% with a product purity of 97.05%, as confirmed by comprehensive physicochemical characterization (XRD, XRF, SEM–EDS, and TGA). To enable predictive control and operational scalability, Gaussian Process Regression (GPR), Bagged Trees (BT), and Artificial Neural Network (ANN) models were developed and refined using Bayesian Optimization. Among all models, ANN exhibited superior generalization performance on unseen data (R^2 = 0.9967, RMSE = 0.1184), accurately capturing nonlinear interactions between process variables and recovery efficiency. Principal Component Analysis further identified alkalinity control as the primary driver of recovery performance, reinforcing the experimental findings. The proposed framework bridges real-brine experimentation with data-driven intelligence, enabling accurate forecasting, informed set-point selection, and minimized co-precipitation risk. This work establishes a replicable, decision-oriented strategy for intelligent brine valorization that supports circular economy principles and advances sustainable mineral recovery in desalination systems.

This work was supported by the Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum and Minerals [Grant number INMW2511].

CAI - D3- P05
Unravelling aspartame-induced activation pathways in the TAS1R2/TAS1R3 receptor

Judith Millan and Rodrigo Martínez
Universidad de La Rioja, Spain

This work centres on the molecular dynamics simulation of a complete model of the human sweet-taste receptor TAS1R2/TAS1R3 bound to the sweetener aspartame. The system has been carefully built to reproduce a realistic biological environment. It includes the full receptor heterodimer embedded in a heterogeneous, asymmetric lipid bilayer mimicking a human cell membrane, fully solvated with explicit water and neutralising ions.
The starting structure is based on a homology-modelled human apo receptor, generated from a chimeric TAS1R2/TAS1R3.[1] Receptor's protonation state and aspartame docking on its binding site were performed by the AI assistant Playmolecule Viewer.[2]
After this, CHARMM-GUI Membrane Builder module[3] was used to insert the complex through a lipidic bilayer of made of POPC phospholipids. The final prepared system consists of around 400,000 atoms and uses CHARMM36m force-field parameters for proteins and lipids, together with CGenFF parameters for the ligand. After geometry preparation, energy minimisation and a multi-step restrained equilibration were carried out, producing a stable, simulation-ready system.
After 500 ns of NPT molecular dynamics simulations several analyses have been performed, such as hydrogen bonds identification, aspartame's, solvent accessible surface area (SASA) or principal component analysis (PCA), to characterise how ligand binding triggers structural changes across the receptor. Domain closure motions or transmitted rearrangements have been investigated to shed light into the sweet taste signal transmission.

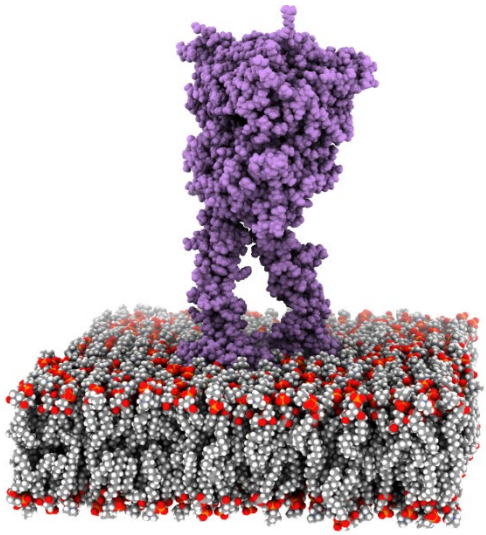

Fig. 1. TAS1R2/TAS1R3 sweet taste receptor inserted in a model lipidic bilayer

Authors acknowledge to "Ministerio de Ciencia, Innovación y Universidades del Gobierno de España" for funding through PID2021-127918NB-I00 project, SGIKER service (UPV/EHU, MICIU-FEDER) for assisting in the computational calculations, and Universidad de La Rioja for its support.

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CAI - D3- P06

Quantum computers for molecular inverse design: The quantum ensemble variational optimization algorithm

Francesco Calcagno[1,2], Delmar G.A. Cabral[3], Ivan Rivalta[1,2], Victor S. Batista[3,4]
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Molecular inverse design is a long-standing challenge in Chemistry with the potential to dramatically accelerate the discovery of novel compounds featuring desired properties.[1] In the past decade, machine learning (ML) and artificial intelligence techniques have gained attention as cutting-edge methods to accelerate screening and generation of functional molecules.[1,2] However, ML models usually rely on large training sets, which may limit unbiased exploration of the chemical space.
Quantum computers natively implement the quantum superposition principle and offer new opportunities for fast exploration of large combinatorial spaces.[3] In the present contribution, we present the Quantum Ensemble Variational Optimization (QEVO) algorithm,[4] a variational quantum algorithm for molecular design. QEVO encodes molecules as Pauli strings using a parametrized quantum circuit. The algorithm iteratively samples ensembles of molecules, whose properties are used to improve the generation by variationally optimizing circuit's parameters (Figure 1).

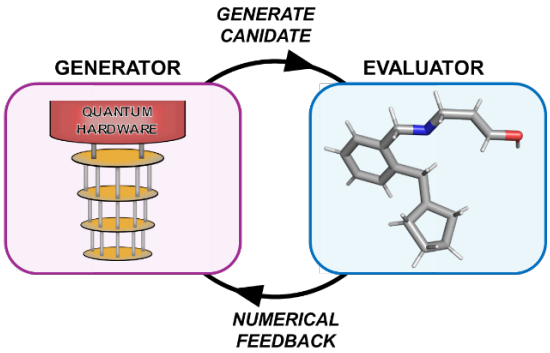

Fig. 1. Workflow of the Quantum Ensemble Variational Optimization (QEVO) algorithm.

We successfully tested QEVO in several molecular design problems with combinatorial complexity up to 2^{160} possible solutions, showing that QEVO correctly samples high-rewarding molecules despite a limited exploration of the total space.[4] Notably, QEVO was able to generate drug-like molecules with anticancer properties, highlighting its potential to pave the way towards new strategies for inverse molecular design using quantum hardware.

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CAI - D3- P08
Automated classification and quantification of pickering emulsion droplets using YOLOv7

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This work presents a deep learning-based strategy for the automatic classification and quantification of Pickering emulsion droplets using the YOLOv7 object detection tool. In complex systems such as Pickering emulsions, the presence of solid stabilizing particles complicates automated detection using conventional image-processing methods [1]. Pickering emulsions stabilized with carbon nanotubes were prepared and imaged by optical microscopy. A curated dataset of micrographs was used to train and validate two YOLO architectures (v4 and v7), with YOLOv7 demonstrating superior performance, particularly in images containing high number of small droplets. The trained model enabled rapid and reliable droplet detection, reducing analysis time from hours to seconds. Following detection, two independent quantification strategies were implemented. The first method estimated droplet diameter directly from bounding box dimensions, while the second applied a segmentation-based approach to more accurately determine droplet boundaries. The full analysis workflow is schematically illustrated in Figure 1. Comparison with manual measurements revealed that the second method achieved a mean error of only 2.74%, corresponding to an overall accuracy of 97.26%. Droplet size distributions confirmed strong agreement between automated and manual measurements, demonstrating that the coupled YOLOv7–segmentation workflow reliably reproduces both average droplet sizes and full distribution profiles, in line with recent deep-learning approaches applied to Pickering emulsions [2]. This study demonstrates the feasibility of applying deep learning tools to complex colloidal systems and highlights their potential to accelerate data extraction from microscopy images. The methodology is transferable to other emulsions and paves the way toward automated characterization platforms.

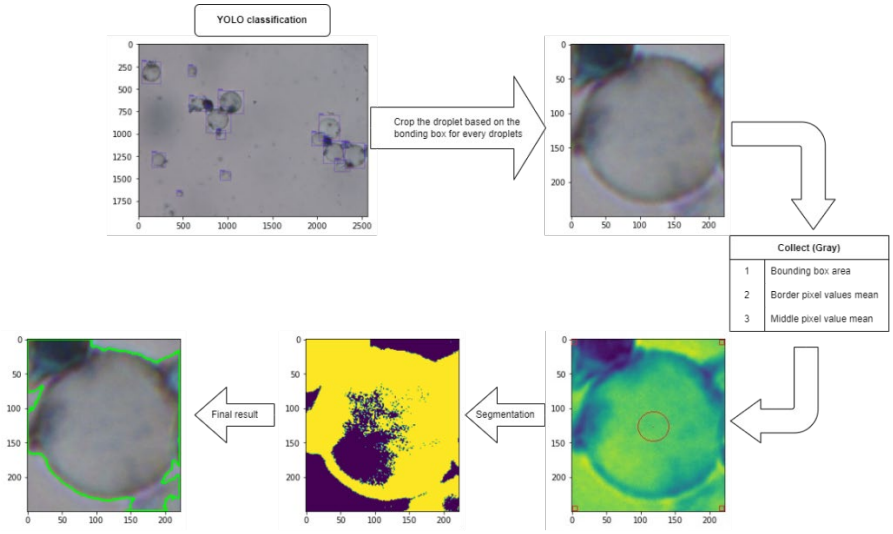

Fig. 1. Second method architecture.

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO UID/00690/2025 (10.54499/UID/00690/2025) and UID/PRR/00690/2025 (10.54499/UID/PRR/00690/2025); SusTEC, LA/P/0007/2020 (10.54499/LA/P/0007/2020). This work was also supported by the project “3D-CARB4E&E – 3D-printed carbon monoliths for energy and environmental applications” (10.54499/2023.18105.ICDT), funded by Programa Inovação e Transição Digital (COMPETE 2030), FCT, I.P., and FEDER, and by ML3DCARB (10.54499/2024.17845.PEX).

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CAI - D3- P09

A reproducible multi-scale computational workflow for DL-methionine in breast cancer targets: DFT, data-driven docking, MD and MM-PBSA validation

Md Wasee Murtuza[1], Mohd. Zaid[1], Manoj Sharma[1], Saleem Javed[1]
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The structural, vibrational, electronic and biological relevance of DL-Methionine (DL-MT), a possible anti-breast cancer agent, were explored by combining experimental FT-IR and UV-Vis spectra with density functional theory (DFT), molecular docking, molecular dynamics (MD) simulations and MM-PBSA binding free-energy estimation. For optimised geometries, harmonic vibrational wavenumbers were computed at the B3LYP/6–311++G(d,p) level, and vibrational spectrum assignments were obtained through normal coordinate analysis in conjunction with Pulay's SQMFF methodology, enabling a precise correlation between simulated and experimental spectral profiles. A comparison of DL-MT frontier molecular orbital (FMO) gaps in dissimilar environments disclosed energy gap values of 5.608 eV (gas), 5.586 eV (water), 5.577 eV (methanol) and 5.581 eV (DMSO), indicating solvent-dependent modulation of reactivity. To predict electrophilic and nucleophilic reactive sites, molecular electrostatic potential (MEP) visualisations were generated in both gas and solvent phases, and Fukui function descriptors were also assessed. Furthermore, AIM, RDG/NCI, DORI, ELF and LOL topological analyses were executed to obtain additional insight into intramolecular stabilisation and electron density localisation behaviour.
In a bid to prioritise biologically relevant targets, molecular docking was conducted against four breast cancer proteins (PDB IDs: 5NWH, 5NQR, 7ULV and 6SZQ), resulting in binding energies of -5.96, -4.51, -4.89 and -4.27 kcal/mol, respectively, and the associated interaction profiles were comprehensively examined. Specifically, 100 ns all-atom MD simulations were performed for the DL-MT complexes of 5NWH and 7ULV (highest docking affinities), and the gmx_MMPBSA protocol was utilised on MD trajectories to determine ΔG_binding values of -20.95 kcal/mol (5NWH) and -0.58 kcal/mol (7ULV). Finally, ADMET predictions and drug-likeness assessments (Lipinski compliance; HIA ≈ 81.6%; logP ~0.15) supported favourable pharmacokinetic behaviour with low predicted toxicity, suggesting DL-MT as a plausible candidate scaffold for follow-up validation[1].

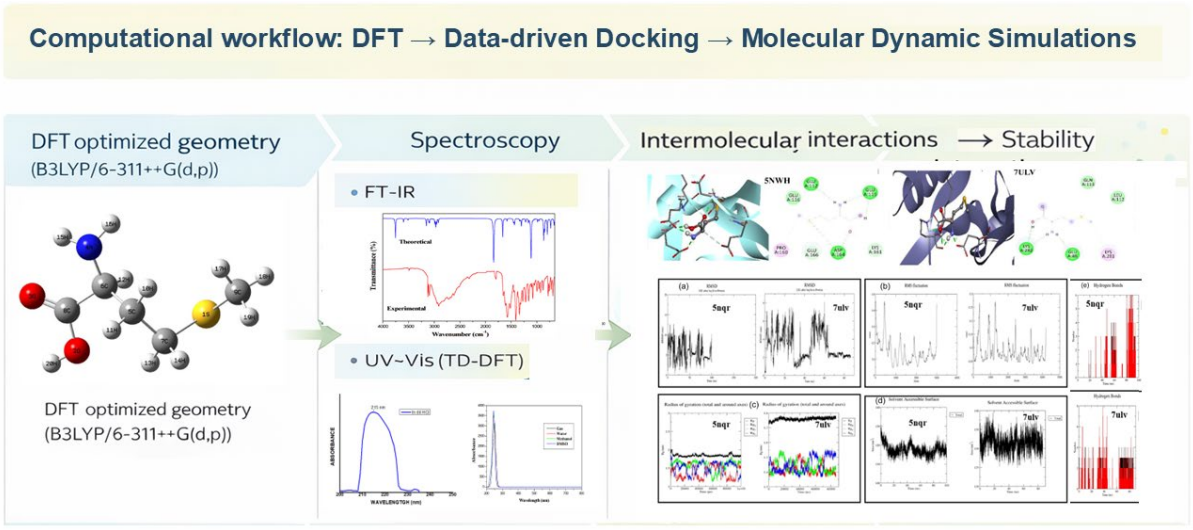

Fig. 2. Computational workflow: DFT, data-driven docking, MD.

Acknowledgement: The original study acknowledges Jamia Millia Islamia (India).

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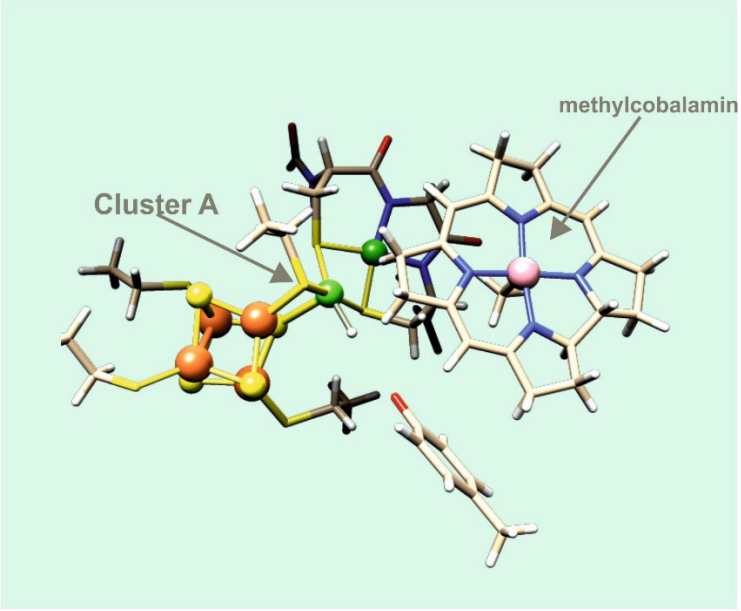
CAI - D3- P10

Mechanism of methylation of A-cluster in coenzyme A synthase by cobalamin. Insight from DFT calculations

Maria Jaworska, Piotr Lodowski
University of Silesia in Katowice, Poland

Acetyl coenzyme A synthase (ACS) catalyzes the synthesis of the acetyl group from the methyl group and carbon monoxide, ultimately leading to the formation of acetyl coenzyme A. The first step in this reaction is the methylation of the nickel ion in the A-cluster of the ACS enzyme. A-Cluster consists of a dinuclear nickel complex linked to iron-sulfur cubane, Fe_4S_4. We propose a mechanism in which the nickel atom on which the reaction occurs, is protonated in the enzyme resting state. When the methylating agent, methylcobalamin, approaches the A-cluster, the proton is transferred to a strong base. We suggest this to be the tyrosine anion, replaced in the calculations by a phenolate anion. To determine the reaction energy, the potential energy surface (PES) was calculated using the DFT/BP86 method. **The potential energy surface** was determined based on the position of the proton and the distance of methylcobalamin from the A-cluster. Calculations were also performed for the same reaction in the presence of a water molecule. The water molecule participating in the reaction facilitates proton transfer and lowers the reaction barrier.



Model of the protonated A-cluster in the presence of methylcobalamin

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The 10th EuChemS Chemistry Congress

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Chemistry Meets Biology & Food Science (CBF)

CBF - D3 - P01

Nanoparticle-based lateral flow immunoassays for detecting marine biotoxins in seafood: A systematic review of trends in development over two decades

Perveen Akhtar [1,2*], Hugh J. Byrne [2], Furong Tian[1,2], Bilal Javed [1,2*]
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Marine and freshwater biotoxins threaten public health and seafood safety due to their tendency to accumulate in fish and shellfish. This systematic literature review summarises findings from 51 peer-reviewed studies published between 2004 and 2025 that focus on nanoparticle-enhanced lateral flow immunoassays (LFIAs) for toxin detection. Gold nanoparticles (AuNPs) were by far the most used label, employed in ~75% of studies, which consistently delivered the lowest limits of detection (LODs) as low as 0.03 ng/ml for okadaic acid detection. Despite increasing concerns over the co-occurrence of multiple toxins, ~88% of the studies were based on single-analyte detection, only ~12% employing multiplexed approaches. Statistical analyses of the studies, namely Kruskal–Wallis, Dunn's post hoc, correlation, and regression analysis, revealed meaningful trends. LODs have significantly improved over time, a marked reduction being observed after 2016. Kruskal–Wallis and Dunn's post hoc tests showed significant differences across variables such as nanoparticle size, assay duration, and toxin recovery. Spearman correlation results identified a moderately significant negative correlation of LOD with publication year ($\rho = -0.458$, $p < 0.001$), and a weaker significant correlation of LOD with assay time ($\rho = -0.301$, $p = 0.018$), while linear regression analysis identified publication year ($R^2 = 0.2441$, $p < 0.0001$) and nanoparticle size ($R^2 = 0.1072$, $p = 0.0264$) as significant predictors of assay sensitivity. Overall, this review underscores the central role of nanoparticle engineering, simplified assay workflows, and optimized design strategies in improving LFIA performance. The findings provide a valuable roadmap for advancing the development of portable, sensitive, and scalable biosensing platforms for marine toxin monitoring and seafood safety surveillance.

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CBF - D3 - P03

Breaking the NMDAR/TRPM4 protein dialogue: Small-molecule disruptors as a novel neuroprotective strategy for ischemic stroke

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Acute ischemic stroke remains one of the leading causes of death and long-term disability worldwide, yet effective neuroprotective therapies are still lacking. For decades, therapeutic strategies focused on global inhibition of *N*-methyl-D-aspartate receptors (NMDARs) to prevent glutamate-driven excitotoxicity.[1] Despite strong preclinical rationale, clinical trials of NMDAR antagonists consistently failed due to severe adverse effects and increased mortality, highlighting the indispensable physiological role of NMDAR signaling in neuronal survival and recovery.[2] Recent discoveries demonstrated that excitotoxic neuronal death is mediated specifically by an extrasynaptic NMDAR/TRPM4 signaling complex. Selective disruption of this protein–protein interaction suppresses pathological signaling while preserving the essential synaptic functions of NMDARs (Figure 1.), establishing the NMDAR/TRPM4 complex as a promising target for next-generation neuroprotective therapies.[3]

However, the chemical space of known disruptors remains extremely limited and is dominated by a narrow class of *N¹*-benzyl-*N¹*-ethylethane-1,2-diamine derivatives with insufficient pharmacokinetic and ADMET characterization.[3] To address this challenge, our project focuses on the medicinal chemistry-driven development of novel small-molecule disruptors of the NMDAR/TRPM4 complex.

Several new compounds have been designed, synthesized, and evaluated *in vitro*. Initial biological studies demonstrated promising activity for selected derivatives, supporting further optimization and structure–activity relationship investigations. By combining synthetic organic chemistry with pharmacological screening, this work aims to expand the repertoire of selective NMDAR/TRPM4 disruptors and advance the development of safer and more clinically viable neuroprotective agents for acute ischemic stroke.

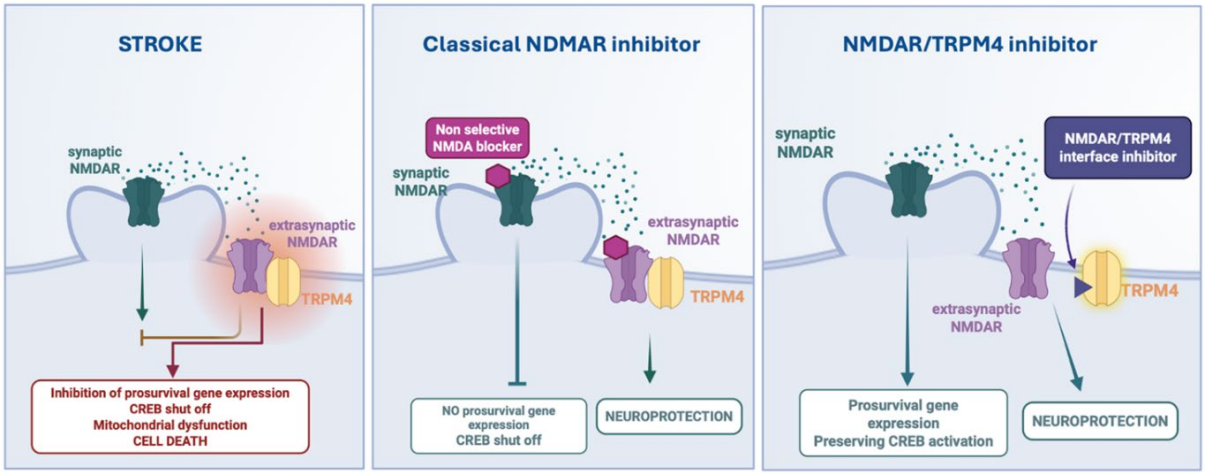

Fig. 1. Classical NMDAR neuroprotection versus selective blockade of NMDAR/TRPM4 interface.

Research funded by National Science Centre, Poland. Projects number 2023/50/E/NZ7/00586 and 2025/57/N/NZ7/02201.

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CBF - D3 - P04
Method validation for the determination of pyridate in agricultural commodities

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Pyridate is a photosynthesis-inhibiting herbicide that suppressed weed growth by blocking electron transport in Phtosystem II. Accoding to CODEX, EC(Europe), EPA(USA), JFCRF(Japan) and PMRA(Canada), maximum residue limits(MRLs) of pyridate are regulated based pyridate, pyridafol(hydrolysis products of pyridate), and pyridafol-O-glucoside(glycosides of pyridafol), expressed as pyridate equivalents, with MRLs ranging from 0.03-10 mg/kg for various agricultural commodities. In Korea, analytical method for pyridate is required as the residue definition is expected to include the parent compound and its metabolites.
In this study, an analytical method verified by the National Institute of Food and Drug Safety Evaluation(NIFDS) was independently validated for the safety management of pyridate and its metabolites. Five representative agricultural commodities(brown rice, potato, soybean, citrus and green pepper) were selected for this method validation. Samples were treated with 1N NaOH and extracted with acetonitrile, followed by acid hydrolysis with 1N HCl at 70℃ and dehydration using $MgSO_4$ and NaCl. The extract was purified using disperse solid phase extraction(d-SPE) kit with anhydrous $MgSO_4$ and C_{18}, and then analyzed by LC/MS/MS. The matrix-matched calibration curves showed good linearity, with coefficients of determination(R^2) greater than 0.99. The limit of detection and the limit of quantification was confirmed to be below 0.003 mg/kg and 0.01 mg/kg, respectively. The method demonstrated acceptable recoveries and precision at three spiked levels(LOQ, 10×LOQ, 50×LOQ, n=3), with recovery values of 89.8-103.6% for pyridate, 80.8-108.8% for pyridafol, and 75.8-96.0% for pyridafol-O-glucoside, and the relative standard deviation was less than 4.7% or less.
These results confirm that the method complies with the residue analysis criteria set forth by the Codex guidelines(Codex Alimentarius Commission, CAC/GL 40). Based on these results, the proposed analytical method has been demonstrated to be suitable for the detection and quantification of pyridate. It can be utilized as a reference method for establishing MRLs.

CBF - D3 - P05

Impact of cation alkyl chain length on the antimicrobial efficacy of 1-alkyl-3-methylimidazolium ionic liquids

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The antimicrobial application of ionic liquids (ILs) have become a significant research focus due to their excellent features such as low volatility, high thermal stability, and tunable properties.[1] This study investigates the antimicrobial efficacy of 1-alkyl-3-methylimidazolium chloride ($C_nMIM[Cl^-]$) and 1-alkyl-3-methylimidazolium tetrafluoroborate ($C_nMIM[BF_4^-]$) ionic liquids at varying alkyl chain lengths against *Staphylococcus aureus* and *Pseudomonas aeruginosa* in both liquid-phase and dry-phase tests on High Efficiency Particulate Air (HEPA) filters. Bactericidal activity increased with the length of the alkyl chain and was concentration dependent. Additionally, bactericidal activity was higher in liquid-phase (figure 1) compared to dry phase with IL coated HEPA filters (figure 2), a disparity which may be attributed to the enhanced solubility and mobility of the ionic liquids in the liquid phase, which allows for more effective interaction with bacterial cells. This could have implications for developing ionic liquid disinfectant formulations for different applications where antimicrobial properties are needed.

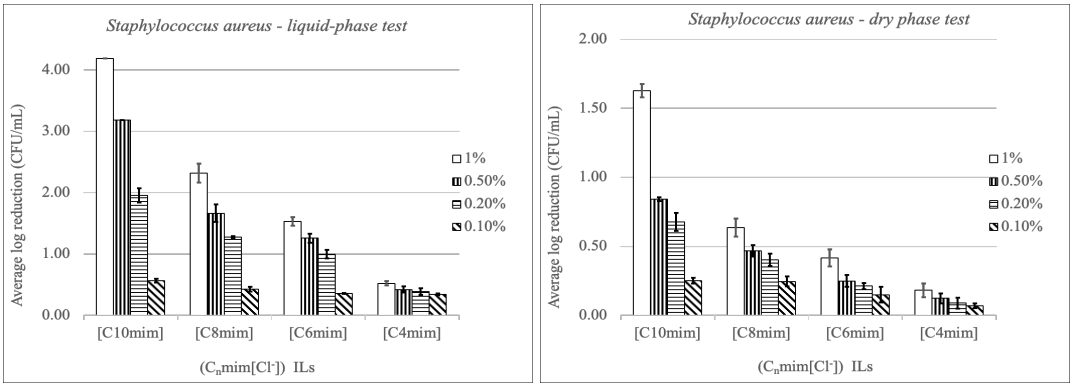

Fig. (1) liquid-phase bactericidal activity (2) dry-phase bactericidal activity of (CnMIM[Cl-]) of varying alkyl chain lengths on *Staphylococcus aureus* bacteria.

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CBF - D3 - P06
What lipid composition best reproduces the biophysical properties of fungal membranes?

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[1]School of Chemistry and Molecular Bioscience, University of Queensland, Brisbane, Australia

Current antifungal drugs lack specificity and selectivity, causing host toxicity, and with the current increasing resistance, there is an urgent need for safer and effective options. Fungal plasma membrane and cell wall components differ from those of other eukaryotes, providing suitable targets for drugs. Lipid vesicles provide a useful model system to understand drug-membrane interactions, where lipid composition and environmental factors can be controlled, but model membranes are only useful if they capture the properties of the cellular membrane.
In this project, we investigate the effects of lipid composition on surface charge and fluidity of vesicles aimed at mimicking fungal membranes. For this, we compare simple lipid vesicles, complex lipid vesicles, and lipid extract vesicles (LEVs) from fungal cells. As expected, ergosterol reduces the fluidity of vesicles composed of zwitterionic phosphatidylcholine lipids (POPC). Interestingly, adding phosphatidylethanolamine lipids (POPE), a zwitterionic lipid sharing the same lipid tail saturation as POPC, significantly reduces the fluidity of PC-ergo vesicles, with a change comparable to that of ergosterol. The addition of anionic lipids further reduces fluidity, indicating that headgroups are as relevant to fluidity as tail saturation or the presence of sterols. A combination of ergosterol, POPE and anionic lipids is required to mimic the fluidity of LEVs. As fungal membranes are enriched in anionic lipids, LEVs showed large negative zeta potentials, and at least 40mol% anionic lipids are required to mimic their surface charge. Surprisingly, fungal cells show much lower zeta potential, indicating that the cell wall shields the negatively charged membrane surface.

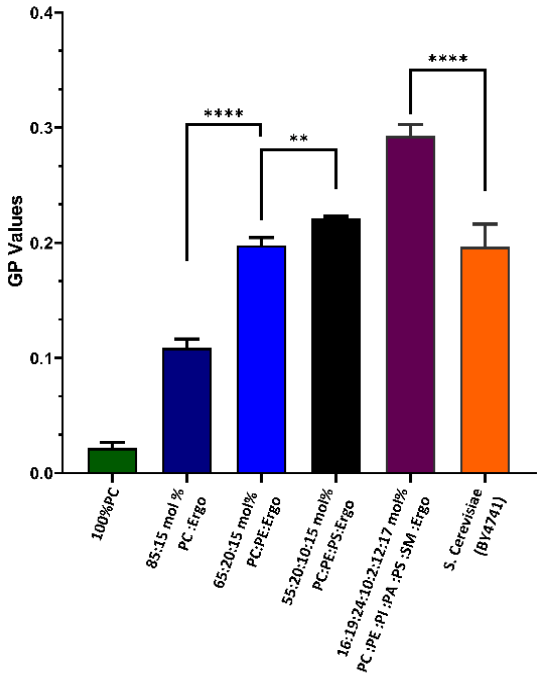

Fig. 1. Generalised Polarisation (G.P.) of the vesicles. Bar plots show Mean ± SEM for at least three replicates. Asterisks indicate **P<0.005, and ****P<0.0001

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Catalyzing New Chemistry Solutions (CCS)

CCS - D3 - P01

Effect of non-metal dopants in self-coupled g-C_3N_4 Van der Waals heterojunctions for efficient photocatalytic tetracycline and PFOA degradation

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Most water treatment applications cannot fully remove Persistent Organic Pollutants (POP) such as antibiotics, microplastics, or per- and fluoroalkyl substances in wastewater streams, leading to their eventual accumulation in water sources and soils. This poses major risks to human health, e.g. due to the evolution of antibiotic-resistant bacteria or the ingestion and build-up of persistent pollutants in the body.[1] A sustainable and affordable method to degrade POP from wastewater is photocatalysis. Photocatalysts effectively harness solar energy to drive pollutant degradation by radical formation and reaction.[2] To date, many photocatalytic systems are based on rare and expensive (noble) metals or are unable to generate sufficiently oxidizing radicals due to their electronic characteristics. To overcome these challenges, our work focuses on synthesizing metal-free self-coupled g-C_3N_4 heterojunctions using an affordable melamine thermal polymerization method with different non-metal dopants. Self-coupled heterojunction formation between pristine and doped g-C_3N_4 is achieved by electrostatic self-assembly. Thereby, Z-scheme systems are formed that can greatly improve light utilization and charge-carrier separation compared to the component materials.[3] The photocatalytic performance of the synthesized materials is investigated for degradation of tetracycline (10 ppm) and perfluorooctanoic acid (PFOA, 100 ppm) as model compounds under simulated sunlight. During these experiments, the effect of different non-metal dopants, the dopant loading, and the ratio of component materials during heterojunction formation is analysed. We show that the photocatalytic activity of g-C_3N_4 photocatalysts is greatly improved compared to the component materials without the need for expensive metal doping.

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CCS - D3 - P02

NiX/Al_2O_3 catalysts for photocatalytic hydrogen production towards intended industrial application

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[1]Thin-film and Nanostructure Electrodeposition Group (GE-CPN) – Universitat de Barcelona, Spain; [2]Consorci per a la Gestió dels Residus del Vallès Oriental, Spain; [3]Solid-state Chemistry Group (QES), Dept. of Inorganic and Organic Chemistry and Institute of Nanoscience and Nanotechnology (IN2UB) – Universitat de Barcelona, Spain

The increasing interest towards renewable feedstocks as green energy sources drives the development of new technological solutions. Hydrogen is an integral part of this sustainable chain, either as a fuel, a chemical reagent, or both. However, its large-scale production still relies mainly on fossil fuels. Photocatalytic production of hydrogen provides an environmentally friendly pathway, which also benefits from bioavailable oxygenated organic species such as ethanol. In any case, catalysts are required to operate under mild conditions and reduce energy costs. Nickel-based catalysts supported on aluminum oxide are a key technological platform for sustainable decarbonization, processes, including hydrogen production, thanks to their moderate cost, good metal dispersion and high thermal stability.

In this study, NiX/Al_2O_3 catalysts, where X = Ø, Cu, Fe or Co, were prepared by a standard wet impregnation method[1] using different metal ratios, while maintaining a constant total metal loading. SEM characterization prior to reaction confirmed the formation of nanoparticles of the active metals on the micrometric Al_2O_3 surface, as well as their homogeneous distribution. The materials were tested for photocatalytic hydrogen production, under 365 nm irradiation at room temperature. Argon was used as the carrier gas, flowing through a Dreschel bottle containing a 9:1 EtOH:H_2O mixture. Of all prepared catalysts, only the Ni-Cu bimetallic system showed H_2 production, which is attributed to the photoactivity of copper oxides. To confirm this behavior, Cu/Al_2O_3 was used as a reference material, while three different Ni/Cu ratios were also tested to evaluate the role of Ni. The $5Ni5Cu/Al_2O_3$ catalyst showed the highest hydrogen production, exceeding that of Cu/Al_2O_3. Finally, stability was assessed, under constant irradiation conditions and during light on/off cyclic experiments. These results highlight the relevance of $Ni\text{-}Cu/Al_2O_3$ catalysts under mild photocatalytic conditions.

Acknowledgements: With the support of the Industrial Doctorates Program of the Dept. of Research and Universities of the Generalitat de Catalunya (project 2022 DI 00035). The authors acknowledge financial support through the AGAUR grant (project 2023 CLIMA 00009), supported by the Dept. of Research and Universities, the Dept. of Climate Action, Food and Rural Agenda, and the Climate Fund of the Generalitat de Catalunya. The authors would also like to thank the CCiT-UB for the use of their equipment.

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CCS - D3 - P03
Heterogeneous catalysts synthesis by electroless deposition for environmental applications

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The development of nanocatalysts greatly benefit heterogeneous catalysis. The synthesis of metallic nanoparticles (NPs) on supports with large surface areas results in a well-dispersed high density of actives sites, thereby enhancing the catalytic activity. Achieving optimal catalytic performance requires precise control over the synthesis process to regulate the metal loading and dispersion. In this regard, electroless deposition enables accurate control over particle size and morphology while allowing metal deposition on a wide variety of supports. The typical composition of an electroless bath contains a metal precursor salt, complexing agents and a reducing agent, all balanced to sustain an efficient autocatalytic reaction[1]. Common reducing agents include phosphates and boranes, whose oxidation often results in the co-deposition of P or B heteroatoms, which may hinder the desired catalytic effect. To avoid this undesired incorporation, hydrazine is used, as its oxidation results in a complete decomposition into H_2 and N_2.
In this work, a Ru and a Ni electroless baths with hydrazine were used to prepare the catalytic materials using carbon-based supports. Regarding Ru bath[2], an optimization study was performed over fluorine-doped tin oxide coated glass (FTO) substrates and followed by UV-vis spectrophotometry. The thin films obtained were characterized by SEM microscopy coupled to EDS, to assess the deposition conditions. Using two carbon substrates, graphite flakes and carbon nanotubes (CNTs) a series of samples at different deposition times were prepared and morphological and compositionally characterized. Prior were successfully oxidized following an acid attack etching combined with ultrafast sonication, to reduce hydrophobicity and facilitate disaggregation, step that subsequently improved the necessary sensitization treatment with Sn and Pd. Optimal deposition conditions were established at 60 and 10 min for Ru and Ni, respectively. The suitability of the prepared materials as catalysts for methane decomposition reaction is currently under evaluation.

Acknowledgements: With the support of the Industrial Doctorates Program of the Dept. of Research and Universities of the Generalitat de Catalunya (project 2022 DI 00035). The authors would like to thank the CCiT-UB for the use of their equipment.

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CCS - D3 - P04

Amino acids as organocatalysts for the electrosynthesis of pinacols from 4-fluoroacetophenone

Claudiu Bostan[1], Martina Bortolami[1], Cristiana Margarita[1], Fabrizio Vetica[2], Marta Feroci[1]

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The growing demand for chiral molecules drives the need for sustainable asymmetric synthesis. Electrosynthesis offers a promising green alternative to classical methods, utilizing selective redox reactions and atom economy to eliminate the need for stoichiometric mediators[1]. The electrochemical reduction of acetophenones is a well-known reaction that can yield either the corresponding alcohol or the dimerization product[2]. This work focuses on the electrochemical dimerization of acetophenones to pinacols. This pathway is particularly challenging compared to alcohol formation, as it requires dual stereoselective control: simultaneous enantioselection and diastereoselection.

To achieve precise stereocontrol, we investigated electrode functionalization via electrografting of microwave-synthesized chiral nanoparticles (L-Pro-NPs) or amino acids, alongside the use of free chiral amino acids in solution.. The successful modification of the Glassy Carbon electrode was confirmed by cyclic voltammetry, as detailed in Figure 1. Specifically, functionalization with chiral nanoparticles enhanced conductivity, whereas the L-Proline layer acted as an insulator, resulting in a marked current peak decrease. Subsequently, comparative electrosyntheses were conducted to optimize the process (results in Table 1), allowing us to reach yields up to 93% with significant variations in diastereomeric ratios.

We achieved exceptional yields and diastereoisomeric control in pinacol formation, highlighting the potential of electrochemical synthesis as a superior alternative to traditional methods. By employing green electrodes, this work marks a significant advancement toward cleaner chemistry, opening new perspectives for the development of more efficient, sustainable, and environmentally respectful synthetic pathways.

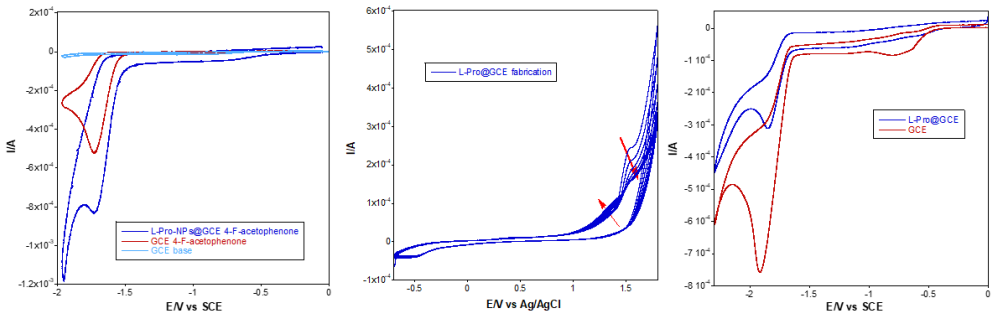

Fig. 1. *Left:* Voltammetry of the ketone with the L-Pro-NPs functionalized GC electrode (in blue). *Right:* Voltammetry of the ketone with the L-Pro functionalized GC electrode (in blue). *Center:* The 10 cycles of L-Pro functionalization.

	Cathode	Solvent	H_2O	Additive	I or E	F/mol	Pinacol (dl/meso)	dl-Pinacol e.r.
1	L-Pro-NPs@GC	CH_3CN	140 eq.	-	-1.7 V	2.5	82% (83/17)	Rac.
2	L-His@GC	CH_3CN	140 eq.	-	-1.85V	1.5	52% (84/16)	51/49
3	L-Ala-L-His@GC	CH_3CN	-	-	-2.20V	1.5	83% (74/26)	51/49
4	GC	DMSO	210 eq.	L-Phe 1 eq.	2 mA	3.0	93% (77/23)	Rac.

Table 1. Cathodic reduction of 4-fluoroacetophenone to the corresponding pinacol

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CCS - D3 - P05

Quantifying structural and dipole–dipole coupling effects in coverage-dependent CO infrared spectra on Pt

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Infrared (IR) absorption bands of adsorbates on catalyst surfaces are widely observed to shift as a function of surface coverage. Such coverage-dependent shifts may originate from two distinct physical mechanisms: adsorption-induced structural deformation of the active site, which modifies the local electronic environment, and dynamic dipole–dipole coupling (DDDC) between neighboring adsorbates, which alters vibrational frequencies without requiring structural reconstruction.

Using CO adsorption on Pt surfaces as a model system, we quantitatively assess both effects. Coverage-induced structural changes of Pt active sites and their impact on CO vibrational frequencies are evaluated using first-principles density functional theory (DFT) calculations combined with machine-learning-based predictions[1]. In parallel, the contribution from dynamic dipole–dipole coupling is investigated by implementing and programmatically extending the semi-empirical model proposed by Brandt[2], enabling quantitative simulations of vibrational coupling as a function of CO coverage, spatial distribution, and nanoparticle morphology.

The relative importance of structural and vibrational coupling effects on coverage-dependent CO frequency shifts is systematically evaluated and compared. Mixed $^{12}CO/^{13}CO$ isotopic adsorption is employed as a probe, both experimentally and theoretically, to disentangle the distinct physical origins of these two mechanisms[3]. This work provides a unified framework for interpreting coverage-dependent infrared spectra of adsorbates on metal catalysts and clarifies the respective roles of structural and vibrational interactions in CO infrared spectroscopy on Pt.

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CCS - D3 - P06

Addition polymerization of norbornene by Cobalt(II) and Palladium(II) complexes ligated *by N, N'*-bidentate iminomethylpyridine derivatives

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The addition polymerization of cyclic olefins has been played as a key technology for synthesizing special polymers with high thermal stability and excellent optical properties. We have synthesized the Co(II) and Pd(II) complexes, namely, **$[L_nMCl_2]$** (M = Co and Pd, L_n = L_A–L_C) supported by iminomethylpyridine derived ligands, such as (E)-N^1,N^1-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine (L_A), (E)-3-methoxy-N-(quinolin-2-ylmethylene)propan-1-amine (L_B), (E)-N-(pyridin-2-ylmethylene)hexan-1-amine (L_C)[1,2]. All complexes were characterized by ^{1}H NMR, ^{13}C NMR, FT-IR and elemental analysis. The X-ray single crystal diffraction revealed that **$[L_ACoCl_2]$** were distorted tetrahedral geometry, while **$[L_BCoCl_2]$** were distorted trigonal bipyramidal geometry. In contrast, Pd(II) complexes, **$[L_BPdCl_2]$** and **$[L_CPdCl_2]$** have shown a distorted square planar geometry around metal center. These complexes were used for the polymerization of norbornene (NB) in the presence of cocatalyst modified methylaluminoxane (MMAO) to give polynorbornene (PNB) at 25°C with high conversion and sterospecific enriched PNB. Specifically, **$[L_ACoCl_2]$** was observed that effectively catalyzed the norbornene with more than 98% conversion and maintained a narrow molecular weight distribution (PDI = 1.13) at 25°C in the presence of MMAO.

This research was supported by the National Research Foundation of South Korea, funded by the Ministry of Education, Science, and Technology (MEST) (Grant No. RS-2023-NR076653 and RS-2025-25415722).

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CCS - D3 - P07

Synthesis and structural characterization of cobalt(II) and palladium(II) complexes bearing *N*-substituted iminomethylpyridine and aminomethylpyridine derivative: Application to ring opening polymerization of *rac*-lactide

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The increasing demand for sustainable polymer materials highlights the need for stereocontrolled metal catalysts for the ring opening polymerization (ROP) of rac-lactide, a renewable monomer used in the production of biodegradable poly(lactic acid) (PLA). To address this challenge, two furfurylamine-derived *N,N'*-donor ligands, (*E*)-1-(furan-2-yl)-*N*-(pyridin-2-ylmethylene)methanamine (L_A) and 1-(furan-2-yl)-*N*-(pyridin-2-ylmethyl)methanamine (L_B) were synthesized through a condensation/reduction sequence and coordinated to anhyrous [$CoCl_2$] and [$Pd(MeCN)_2Cl_2$] to afford a series of metal complexes **[L_nMCl_2]** (L_n = L_A and L_B; M = Co and Pd).

The ligands and resulting complexes were characterized using ^1H and ^{13}C NMR spectroscopy, elemental analysis, FT-IR spectroscopy, and single crystal X-ray diffraction (SCXRD). Preliminary structural results indicate the formation of well-defined metal–ligand architecture, specifically by SCXRD analysis is being refined to elucidate the coordination environments, the influence of ligand frameworks, and metal centers on complex structure.

Catalytic evaluation is being conducted following activation with LiO^tBu to generate *in situ* metal alkoxide species known to initiate ROP. ROP studies at 0 °C and 25 °C aim to assess initiation efficiency, monomer conversion, and stereoregularity. Preliminary results indicate that the ligand backbone plays a significant role in modulating polymerization behavior, likely through steric and electronic effects at the metal center.

By integrating ligand design, coordination chemistry, and catalytic performance, this study seeks to identify molecular factors that promote efficient and selective lactide polymerization. The findings are expected to contribute to the rational development of sustainable transition metal-based catalysts for biodegradable PLA production and to inform future catalyst design in polymer chemistry.

This research was supported by the National Research Foundation of South Korea, funded by the Ministry of Education, Science, and Technology (MEST) (Grant No. RS-2023-NR076653 and RS-2025-25415722).

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CCS - D3 - P08
Chiral CN-palladacycles as precatalysts for alkoxycarbonylation of styrene derivatives

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Carbonylation reactions are powerful tools for the synthesis of carbonyl-containing compounds such as esters, amides, aldehydes, ketones, and acids, which are ubiquitous in pharmaceuticals and fine chemicals. Palladium-catalyzed alkoxycarbonylation of olefins provides an efficient route to ester derivatives; however, achieving high regio- and stereocontrol remains challenging. Palladacycles have emerged as robust and well-defined precatalysts due to their air and moisture stability and controlled ligand environments. While phosphine-stabilized CN-palladacycles are known to promote alkoxycarbonylation with high regioselectivity, the development of chiral variants capable of inducing asymmetry is still largely unexplored.
Herein, we report the synthesis of chiral CN-palladacycles obtained via ortho-palladation of chiral imines and their preliminary evaluation in alkoxycarbonylation reactions using alcohols as nucleophiles under acidic CO conditions. The chiral palladacycles were obtained in moderate to good yields (typically >80%) and displayed high stability toward air and moisture. Their structures were confirmed by multinuclear NMR spectroscopy, IR spectroscopy, and mass spectrometry.
Preliminary catalytic studies in the alkoxycarbonylation of styrene derivatives revealed that a representative chiral complex achieved a conversion of approximately 67% while maintaining a pronounced regioselectivity toward the branched ester product (B:L ≈ 90:10). Importantly, the introduction of chiral substituents on the imine fragment did not compromise catalytic activity or regioselectivity, indicating that the chiral environment is well accommodated within the catalytic framework. These results represent an initial step toward the development of asymmetric alkoxycarbonylation processes based on chiral CN-palladacycle precatalysts. Ongoing work is focused on expanding the substrate scope and further optimization to evaluate potential asymmetric induction.

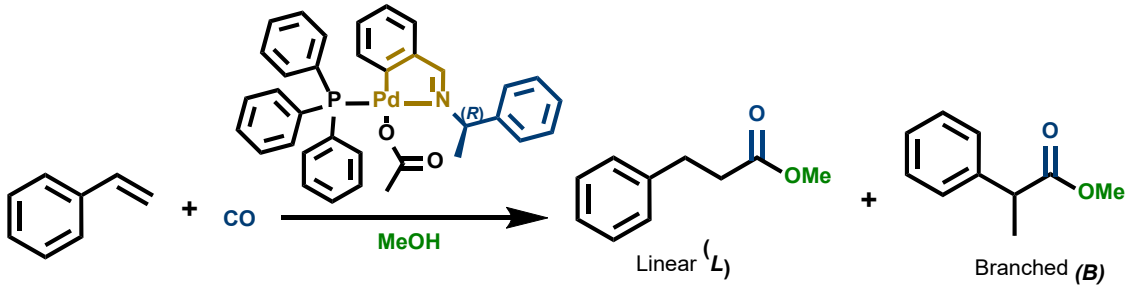

Fig. 1. Representative alkoxycarbonylation of styrene catalyzed by a chiral CN-palladacycle.
*Reaction conditions: Styrene (0.34 mmol), Pd complex (1 mol%), MsOH (5 mol%), LiCl (8 mol%), 5 mL of CH2Cl2: ROH (4:1, v/v), CO (400 psi), 80 °C, 12 h.

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CCS - D3 - P09

Enhanced photocatalytic degradation of phenols using g-C_3N_4-supported phthalocyanine catalysts

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Phenolic compounds are widely recognized as persistent organic pollutants frequently detected in industrial wastewater, posing serious environmental and human health risks [1]. In this study, novel phthalocyanine-based photocatalysts supported on graphitic carbon nitride (g-C_3N_4) were developed to enhance the photocatalytic degradation of phenols under visible-light irradiation. The catalysts were synthesized via a rational molecular design strategy employing bio-derived aromatic precursors, with the aim of improving light-harvesting capability and charge transfer efficiency.

The successful synthesis and structural integrity of the g-C_3N_4-supported phthalocyanine catalysts were confirmed using various spectroscopic and physicochemical characterization techniques [2]. Photocatalytic performance was systematically evaluated through the degradation of phenol in aqueous media, and the effects of key operational parameters—including irradiation time, catalyst dosage, and initial phenol concentration—were thoroughly investigated [3].

The hybrid photocatalysts exhibited significantly enhanced photocatalytic activity compared to unsupported phthalocyanine systems. This improvement is attributed to superior visible-light absorption, efficient charge separation, and accelerated interfacial electron transfer facilitated by the g-C_3N_4 support. Furthermore, the results indicate that both the molecular structure of the phthalocyanine and the nature of the central metal ion play critical roles in determining photocatalytic efficiency [4].

Overall, this study demonstrates that g-C_3N_4-supported phthalocyanine photocatalysts represent a promising and sustainable approach for the efficient removal of phenolic pollutants from water.

This study was supported by The Research Fund of Karadeniz Technical University (Project no: 16562).

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CCS - D3 – P10
Preparation of ferrocene thioamides and their mechanochemical C-H arylation

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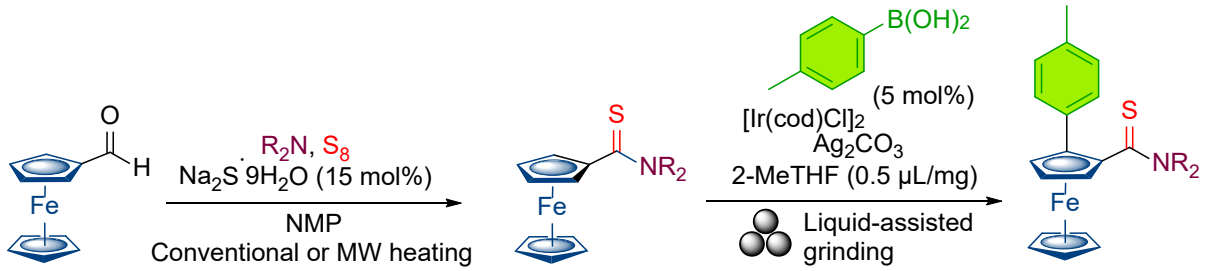
A diverse series of ferrocene thioamides was obtained by the multicomponent Willgerodt-Kindler reaction of ferrocenecarboxaldehyde with various primary or secondary amines and sulfur in the presence of $Na_2S{\cdot}9H_2O$ (Scheme 1). Comprehensive solvent screening shows that amide-type solvents greatly enhance the reaction. On the other hand, this reaction is constrained by the steric hindrance of the bulky amine substrates. While conventional heating is sufficient for secondary amines, primary amines give better results under microwave irradiation at elevated temperature. Investigation of the reaction mechanism by NMR kinetic measurements as well as UV-Vis spectroscopy revealed that sodium sulfide serves as a promoter and not as a catalyst.[1] Selected ferrocene thioamides were subsequently used as substrates for the study of mechanochemical C-H arylations. C-H activations represent modern methods of organic synthesis, which are currently receiving great attention due to their economic and environmental benefits. A major disadvantage of many C-H activation reactions is their long reaction times, often ranging from 12 to 24 hours. This limitation can be overcome by mechanical grinding in a ball mill, which often accelerates the reaction and improves the product yields. Mechanochemical Ir-catalyzed C-H arylation of ferrocene thioamides using *p*-tolylboronic acid as an aryl source and Ag_2CO_3 as an oxidizing agent furnishes a range of *ortho*-arylated thioamides (Scheme 1). Among the LAG additives tested, 2-MeTHF proved to be the most suitable option. The reaction requires heating the milling jar to a temperature of 60 °C. For this purpose, a heating bandage connected to a thermostat is used.



Scheme 1. Synthesis of ferrocene thioamides followed by mechanochemical C-H arylation.

This work was supported by the Slovak Grant Agency VEGA, grant no. 1/0464/25.

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CCS - D3 – P11

Iron-porphyrin catalyzed deaminative hydrobenzylation of alkenes using redox-active pyridinium salts

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All-carbon quaternary centres are highly valued motifs in drug discovery, as increasing the fraction of sp^3 carbons correlates with improved clinical success[1]. These centres impart conformational rigidity and molecular complexity, enhancing aqueous solubility, metabolic stability, and selective protein binding through their three-dimensionality relative to sp^2-rich scaffolds[2]. Although prevalent in natural products and natural product-derived drugs[3], quaternary carbons remain synthetically challenging to access using traditional two-electron polar disconnections, which often require harsh conditions and multistep sequences that limit efficiency and functional group tolerance.

Radical cross-coupling strategies have begun to address these challenges. MacMillan's S_H2 platform enabled selective coupling of primary and tertiary carbon-centred radicals under mild conditions using an iron–porphyrin catalyst[4]. Subsequent incorporation of metal-hydride hydrogen atom transfer (MHAT) catalysis by Baran and Shenvi[5] allowed direct generation of tertiary radicals from alkenes. Coupling with diverse primary radical precursors — including redox-active esters, benzyl bromides, 1,4-dihydropyridines, and alcohols[5–8] — has provided new approaches to $C(sp^3)$–$C(sp^3)$ quaternary carbon formation.

Here, we report a deaminative hydrobenzylation strategy that merges MHAT with a reductive pathway using N-benzylpyridinium salts and a commercially available iron–porphyrin catalyst. This approach simplifies precursor preparation and avoids specialized catalysts. The method enables efficient $C(sp^3)$–$C(sp^3)$ bond formation between alkenes and benzylic amines across 45 examples, delivering 25–92% isolated yields. Mechanistic studies, including radical probes and spectroscopic analysis, support a radical-intermediate pathway involving EDA complex formation.

The operational simplicity, broad scope, and mechanistic insight of this platform highlight its utility for late-stage functionalisation and rapid construction of densely substituted, drug-relevant scaffolds.

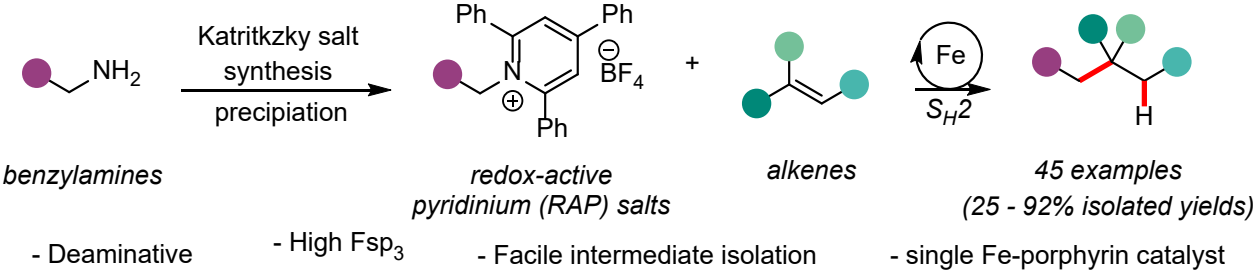

Fig. 1. Deaminative hydrobenzylation of alkenes via MHAT/S_H2 catalysis. Benzylic amines are converted to redox-active N-benzylpyridinium salts, which undergo iron–porphyrin-catalyzed radical cross-coupling with alkenes to furnish all-carbon quaternary centers.

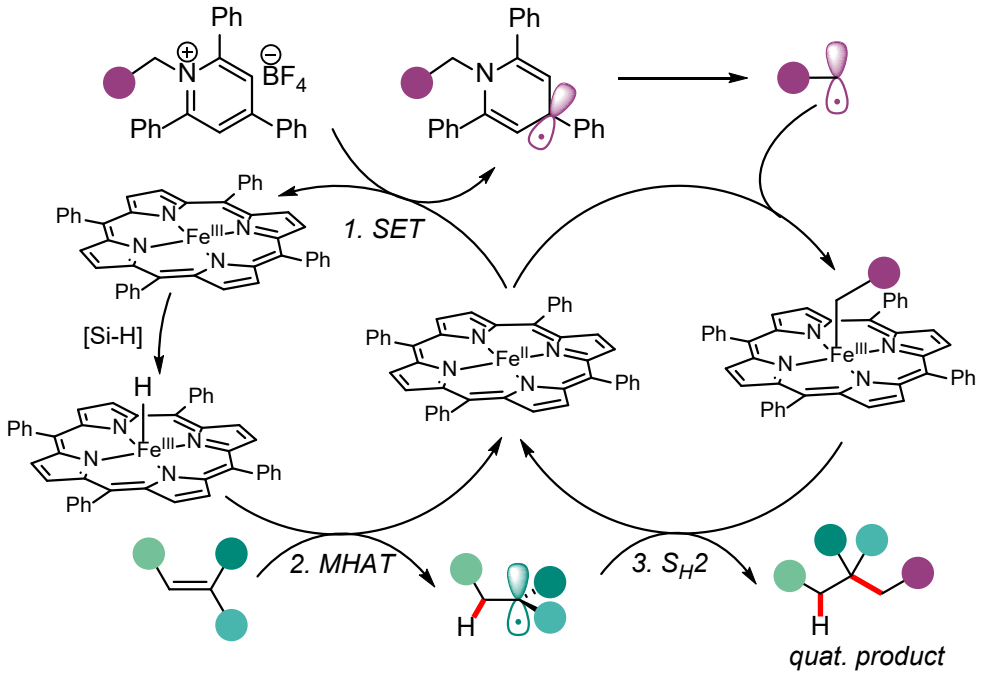

Fig. 2. Proposed mechanism showing SET activation of the pyridinium salt, MHAT generation of a tertiary radical, and S_H2 cross-coupling to form the quaternary carbon product.

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CCS - D3 – P12
Understanding and tuning the reduction of nitro-compounds in water at carbon surfaces

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Amine compounds play a crucial role in pharmaceutical chemistry and many areas of the chemical industry, as they are key structural motifs in a wide range of biologically active molecules and functional materials. Therefore, understanding the synthesis of amine group is essential. Both aliphatic and aromatic nitro compounds are reduced readily at carbon electrodes in aqueous electrolyte. Reduction of nitroarenes typically gives the amine (aniline) product, via a hydroxylamine intermediate. This has been exploited in hydrogenation (bio)catalysts that use a H_2-activating site (e.g. the hydrogenase enzyme) to supply electrons to the carbon surface, so that nitro compounds can be reduced at the carbon.[1] A similar mechanism can occur with Pd/C catalysts, where Pd catalyzes H_2 oxidation, and the carbon is responsible for nitro-group reductions.[2] Although the carbon is typically considered just a *support*, it actually appears to have an electrocatalytic role, since different carbon materials can tune the onset potential for nitro reduction. This project explores electrocatalytic reduction of model nitro compounds, nitrobenzene, nitrophenol and nitrohexane, at different carbon surfaces to evaluate onset potential, and selectivity for hydroxylamine to amine. This will pave the way for a computational study to evaluate interactions of nitro compounds with the carbon materials and the mechanism for their reduction. This poster presents electrochemical analysis and preliminary plans for the computational work.

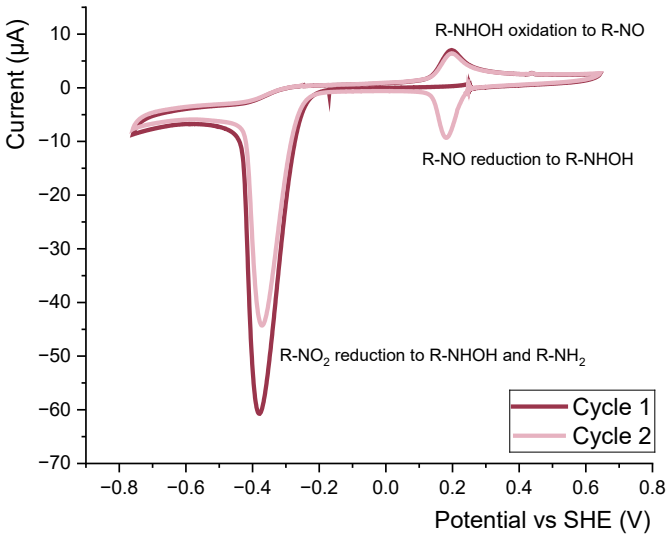

Fig. 1. Cyclic voltammogram of 1 mM nitrobenzene in sodium phosphate buffer (50 mM, pH=6.0) at a pyrolytic graphite 'edge' working electrode, scan rate 10 mV/s at 25℃.

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CCS - D3 – P13
Utilization Of 2D transition-metal dichalcogenide supports for rhodium-catalyzed hydroformylation

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Two-dimensional transition-metal dichalcogenides (TMDs) have recently attracted increasing attention as catalyst supports due to their layered structure, tunable electronic properties, and strong metal–support interactions enabling stabilization of highly dispersed active species. In this work, we investigate the utilization of MoS_2 [1]and WS_2 [2]as supports for rhodium-based heterogeneous catalysts for styrene hydroformylation, aiming to develop recyclable catalytic systems with performance approaching that of homogeneous rhodium complexes.
Rhodium catalysts with loadings between 0.5 and 10 wt.% were prepared by wet impregnation under different temperatures, followed by optional thermal treatments. The influence of preparation conditions on catalyst structure and performance was studied using XRF, XRD, N_2 physisorption, SEM, TEM, and temperature-programmed desorption of pyridine. Both MoS_2- and WS_2-based catalysts showed formation of highly dispersed Rh nanoparticles with typical sizes below 5 nm, located on the surface of layered sulphide supports. The layered morphology together with the presence of sulphur vacancies enables strong anchoring of Rh species and provides an electronic environment that can influence key steps of the hydroformylation mechanism.
Catalytic testing in styrene hydroformylation (CO/H_2, 3 MPa, 100 °C) revealed that both supports allow achieving high aldehyde selectivity around 80 %, comparable to the homogeneous Wilkinson catalyst, while preserving the advantages of heterogeneous systems such as easy separation and potential reuse. Optimal performance was obtained for catalysts with Rh loading ≥ 2 wt.% prepared under mild conditions. In contrast, high-temperature calcination led to partial sulphur loss, formation of oxide phases, increased surface acidity, and a higher tendency toward oligomerization and hydrogenation side reactions, resulting in decreased aldehyde selectivity.
The results demonstrate that layered TMD materials act as ligand-like supports that stabilize catalytically active Rh species and confirm that 2D supports represent a promising platform for designing selective heterogeneous hydroformylation catalysts.

This research was supported by the Czech Science Foundation (GACR No. 23–08083M) and by the institutional support Dagmar Procházková Fund provided by University of Chemistry and Technology in Prague.

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CCS - D3 – P14

Atroposelective access to oxicam-inspired axially chiral benzopyrano[1,2]thiazinone S,S-dioxides via oxidative NHC catalysis

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Atropisomerism, a stereochemical phenomenon arising from restricted rotation around σ bonds, can afford configurationally stable axially chiral molecules. Owing to their importance in asymmetric catalysis, drug discovery, and functional materials, the development of efficient atroposelective synthetic strategies remains a significant challenge. In particular, the catalytic construction of a stereogenic C–C axis within densely functionalized and polycyclic systems requires precise control over both reactivity and conformational stability[1]. In this context, N-heterocyclic carbenes (NHCs) have emerged as powerful organocatalysts, enabling diverse transformations through both umpolung and non-umpolung reactivity modes. Their unique ability to generate reactive intermediates under mild conditions, combined with tunable steric and electronic properties, allows for precise control – yet their application in constructing axially chiral benzothiazine-based scaffolds has remained unexplored[1,2].

Herein, we present an atropoenantioselective oxidative NHC-catalyzed approach to benzopyrano[1,2]thiazinone S,S-dioxides bearing a stereogenic C–C axis. The strategy is based on an oxicam-inspired benzothiazine 1,1-dioxide core, a scaffold structurally related to the oxicam class of nonsteroidal anti-inflammatory drugs (NSAISs)[3,4]. By introducing axial chirality into this framework, we expand beyond conventional point-chiral oxicam-derived systems and access structurally complex polycyclic architectures. The developed methodology provides products with high enantioselectivity (up to 92% ee), demonstrating effective stereocontrol under oxidative NHC catalysis.

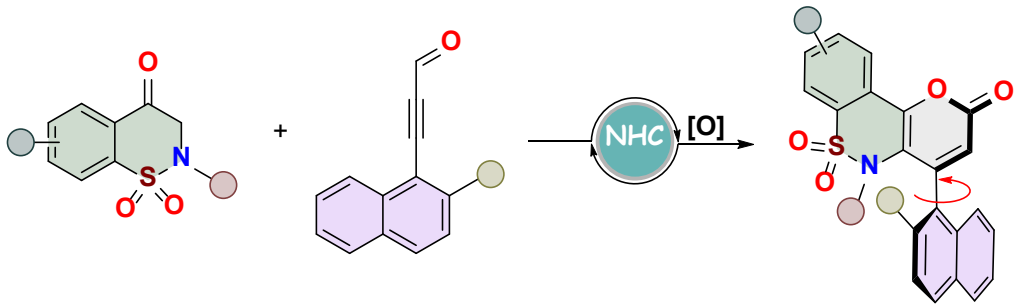

Fig. 1. NHC-catalyzed synthesis of tricyclic α-pyranones with chiral C–C axis.

Project co-financed by the National Science Center within the framework of the program PRELUDIUM BiS 4 (UMO – 2022/47/O/ST4/02432).

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CCS - D3 – P19

Novel Bi_3O_4Br/TiO_2NB/glucose hydrochar for photocatalytic degradation of pharmaceuticals

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To harness their synergistic effects, novel ternary composite photocatalysts containing Bi_3O_4Br, TiO_2 nanobelts, and glucose hydrochar were developed using one step and two steps hydrothermal synthesis for the visible-light degradation of pharmaceuticals. Hydrochar, despite its lower energy requirement, defect-rich structure, abundant oxygen-containing functional groups and effective role as an electron shuttle that could enhance charge transfer, it has remained underexplored compared to the biochar component (1-2). Hence in this work, we explored the unique importance of the one-step versus two-step hydrothermal synthesis. Different ratios (5, 10, 15, and 20%) of the glucose hydrochar was used to synthesize the Bi_3O_4Br/TiO_2NB/GH photocatalysts. In the one-step hydrothermal method, glucose, TiO_2NB, and Bi_3O_4Br precursors were combined and hydrothermally treated simultaneously, whereas in the two-step hydrothermal method, glucose hydrochar was first formed on TiO_2NB, followed by a second hydrothermal step to grow Bi_3O_4Br on the pre-formed TiO_2NB/GH composite. Extensive characterization of the prepared materials revealed that, the two-step method promoted Bi_3O_4Br nanosheet growth on hydrochar. Overall, the incorporation of hydrochar into the Bi_3O_4Br/TiO_2NB photocatalyst primarily enhanced interfacial electronic coupling and charge-transfer efficiency (Fig.1). DRIFT spectroscopy revealed abundant oxygen-containing functional groups on hydrochar, which facilitate interfacial interactions and electron shuttling. These interactions were directly confirmed by XPS through consistent negative shifts in Ti 2p, Bi 4f, Br 3d, and O 1s binding energies, evidencing strong electronic coupling. UV-Vis DRS showed enhanced visible-light absorption without significant bandgap alteration, attributed to hydrochar's light-harvesting capability The two-step 10% photocatalyst achieved the highest degradation efficiency (91%) at natural pH under visible LED irradiation. Scavenger tests (Fig.2) and EPR identified the dominant reactive species, while selective Pt and MnO_x photodeposition confirmed a Z-scheme mechanism with hydrochar acting as an effective electron mediator. The photocatalyst also exhibited potential for treating real pharmaceutical wastewater.

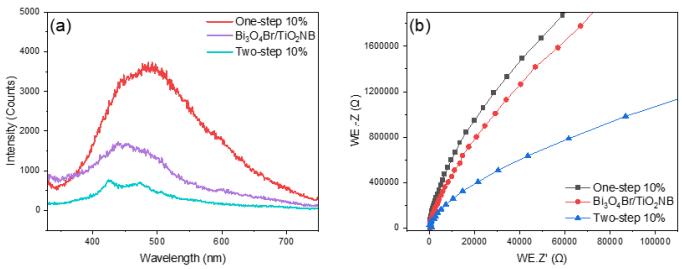

Fig. 1. (a) Photoluminescence and (b) Electrochemical impedance analysis

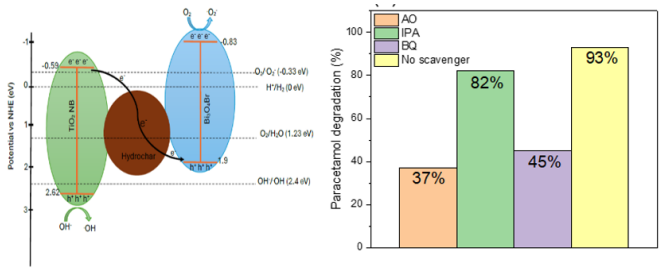

Fig. 2. Proposed mechanism and scavenger analysis

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CCS - D3 – P20

V_2O_5/CeO_2 catalyst for selective oxidative C-N coupling of amines and alcohols into imines

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The oxidative coupling of alcohols and amines to produce imines, commonly known as Schiff bases, is an important transformation in the synthesis of fine chemicals, dyes, insecticides, and pharmaceuticals. Traditional methods often rely on noble metal catalysts, which are expensive, less sustainable, and encounter difficulties in catalyst recovery and reusability. CeO_2 is an alternative and promising support due to its unique redox properties and high density of oxygen vacancies that facilities the oxidative C-N coupling of amine and alcohol. In the work V_2O_5/CeO_2 catalysts were studied to enhance its catalytic activity. The synthesized catalysts were systematically characterized and correlated with its catalytic performance. Among the catalysts screened, the V_2O_5/CeO_2 catalyst exhibits 97.0 of benzyl alcohol conversion and 100.0% of selectivity for N-benzylideneaniline. Further, the N-benzylideneaniline product was purified and isolated by column and thin-layer chromatography.

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CCS - D3 – P21

A sustainable MgO@EDTA@Ag nanocatalyst for eco-friendly xanthene formation and efficient rhodamine B degradation

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The development of environmentally benign and high-performance catalytic systems is essential for advancing green chemistry and effective environmental remediation. In this study, a MgO@EDTA@Ag nanocomposite was successfully synthesised and employed as a multifunctional heterogeneous catalyst for the sustainable synthesis of xanthene derivatives and the efficient degradation of Rhodamine B dye. The presence of EDTA provided strong surface coordination sites, facilitating effective anchoring of silver nanoparticles and enhancing electron transfer processes and reactive species generation, which are crucial for catalytic activity. The synthesised nanocatalyst was comprehensively characterised using XRD, XPS, FESEM, TEM, FTIR, EDAX, TGA, nitrogen adsorption-desorption studies, and BET analysis. These techniques confirmed the successful formation of the nanocomposite, along with its structural stability, favourable surface morphology, high thermal stability, and large specific surface area. The MgO@EDTA@Ag nanocatalyst exhibited excellent catalytic performance, as supported by favourable green chemistry metrics, including a low E-factor (0.23), a low process mass intensity (PMI=1.23), a high reaction mass efficiency (RME=90.06%), and a high carbon efficiency (CE=90%). Additionally, the catalyst demonstrated good recyclability and environmental compatibility, highlighting its suitability for sustainable chemical synthesis and wastewater treatment applications. Notably, in photocatalytic degradation studies, the catalyst achieved 96% degradation of Rhodamine B within 60 minutes using only 0.02 mg of catalyst in 2 mL of dye solution, demonstrating its high efficiency and potential for practical environmental remediation.

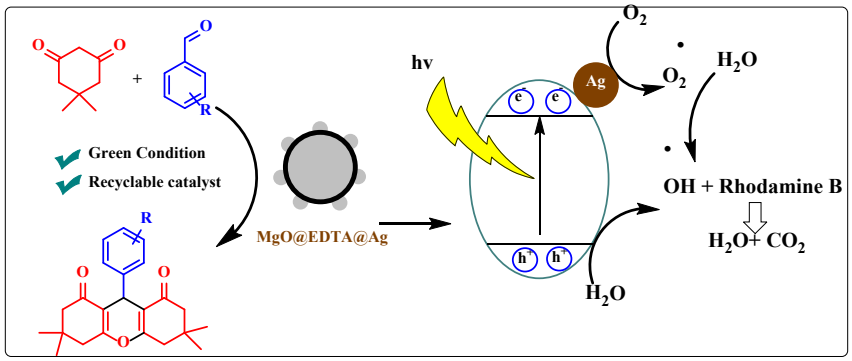

Fig. 1. Graphical abstract

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CCS - D3 – P23

From isolated Rh single atom catalytic sites to cooperative single atom ensembles: Tuning catalytic pathways in CO_2 and ethanol interactions

Ayse Dilay Erdali[1], Yusuf Kocak[1], Kaan Karaca[1], Messaoud Harfouche[2], Ahsan Jalal[1], Ahmet Kerim Avcı[3], and Emrah Ozensoy[1,4*]

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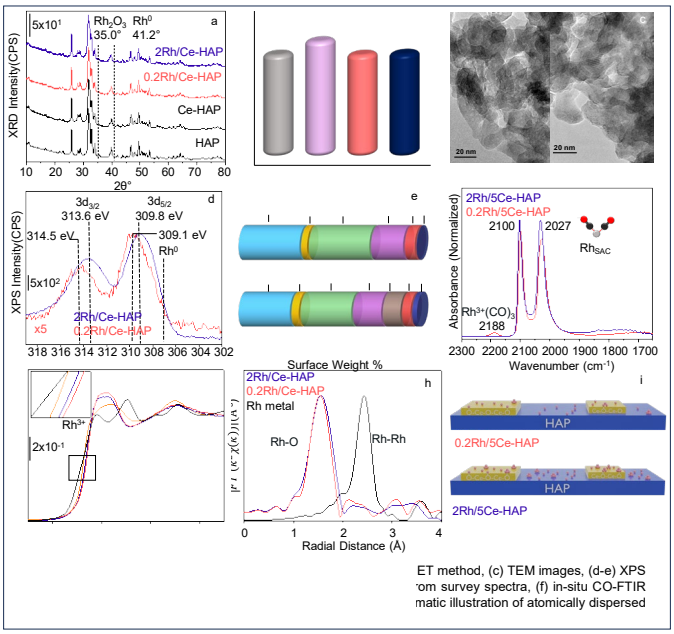

ET method, (c) TEM images, (d-e) XPS om survey spectra, (f) in-situ CO-FTIR matic illustration of atomically dispersed

Co-adsorption of ethanol and CO_2 on Rh single-atom catalysts (SACs) with different metal loadings (0.2 wt% and 2 wt% Rh) supported on ceria-promoted hydroxyapatite (Ce-HAP) in relevance to ethanol dry reforming reaction ($C_2H_5OH(g) + CO_2(g) \rightarrow 3CO(g) + 3H_2(g)$) was investigated via multimodal spectroscopic, imaging and diffraction techniques (i.e., in-situ FTIR, TPD, XANES, EXAFS, XPS, TEM, and XRD). Upon ethanol and CO_2 adsorption at 50 °C, Rh^{3+} species on 0.2Rh/Ce-HAP led to the formation of ethoxides, carbonates, and bicarbonates. Increasing the temperature to 350 °C resulted in oxidation of adsorbed ethoxide species to acetate. In contrast, 2Rh/Ce-HAP catalyst exhibited relatively reduced $Rh^{(3-x)+}$ and $Ce^{(4-y)+}$ sites as opposed to 0.2Rh/Ce-HAP, where 2Rh/Ce-HAP facilitated ethoxide decomposition to acetaldehyde, CO, and CH_4 via C-C/C-H bond activation. This behavior suggested a noticeable difference in the reactivity patterns where a catalytic route including ethoxide oxidation to acetate is replaced with an alternative route comprised of ethoxide dehydrogenation and C-C/C-H bond scission with increasing Rh loading. Our results indicate that while reactivity of SACs at low loadings may be predominantly dictated by isolated single Rh sites, at extremely high loadings, cooperative action of multiple Rh SAC sites located in proximity of Rh clusters which are generated in-situ can lead to significant differences in catalytic reaction mechanisms. Accordingly, the current findings provide valuable molecular-level insights into the design of novel SAC catalysts with varying catalytic selectivity and reactivity as a function of platinum-group-metal (PGM) loading.

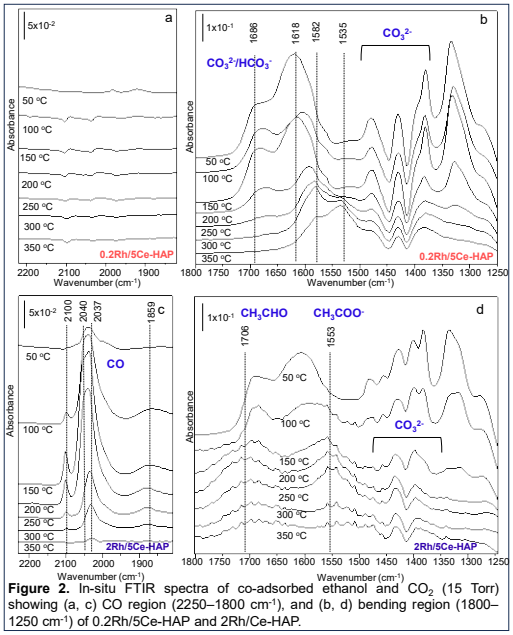

Figure 2. In-situ FTIR spectra of co-adsorbed ethanol and CO_2 (15 Torr) showing (a, c) CO region (2250–1800 cm^{-1}), and (b, d) bending region (1800–1250 cm^{-1}) of 0.2Rh/5Ce-HAP and 2Rh/Ce-HAP.

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CCS - D3 – P25

New N-heterocyclic carbene platinum complexes – synthesis, characterisation and catalytic activity.

Anna Smoczyńska[1], Sylwia Ostrowska[1], Steven P. Nolan[2] Cezary Pietraszuk[1]

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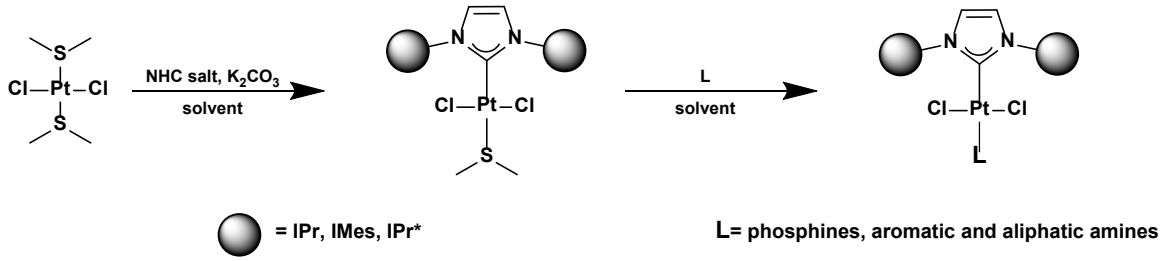
Platinum complexes have attracted considerable interest for many years due to their unique properties and applications in catalysis.[1]

In particular, platinum complexes bearing N-heterocyclic carbene (NHC) ligands exhibit notable catalytic activity in processes such as hydrometallation, dimetallation, hydroamination.[2] Appropriate ligand design can not only enhance the catalytic efficiency of platinum but also enable precise control over reaction selectivity.

This work focuses on the synthesis, characterization, and investigation of the catalytic activity of the N-heterocyclic carbene platinum complexes. In particular, the aim of the syntheses was to obtain complexes with sterically bulky carbene ligands.

The synthesis is based on an approach consistent with the principles of green chemistry, leading to the formation of the [$PtCl_2$(NHC)(DMS)] complex[3], followed by a ligand substitution step in which the DMS ligand is replaced by another ligand.



Drawing 1 General synthesis of platinum complexes[3]

The synthesized complexes were characterized using spectroscopic techniques as well as single-crystal X-ray diffraction analysis. The resulting complexes are applied in catalysis and are also investigated for their potential biological properties. Their catalytic performance was evaluated in Suzuki[4] and selected other coupling reactions.

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Energy, Environment & Sustainability (EES)

EES - D3 - P01
Greener synthetic approaches to the synthesis of quinoxaline derivatives

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Quinoxaline derivatives are an important class of nitrogen-containing heterocycles with applications in medicinal chemistry, materials science, and fluorescence-based sensing. However, many reported synthetic routes rely on hazardous solvents, excess reagents, and energy-intensive conditions, limiting their sustainability and suitability for instructional laboratories. This work explores greener synthetic strategies for the preparation of quinoxaline derivatives while engaging undergraduate students in environmentally responsible research.

A series of quinoxaline derivatives was synthesized via the condensation of substituted *o*-phenylenediamines with 1,2-dicarbonyl compounds using both traditional and green chemistry–inspired approaches. Conventional methods employing organic solvents and prolonged heating were compared with modified protocols that incorporate ethanol as a greener solvent, reduced reagent loading, and milder reaction conditions. In select cases, less hazardous reagents were evaluated as substitutes for commonly used alternatives. Reaction progress was monitored by thin-layer chromatography, and products were characterized using infrared spectroscopy, nuclear magnetic resonance spectroscopy, and UV–visible spectroscopy.

Comparative analysis demonstrated that the greener methods provided comparable or improved yields while significantly reducing solvent toxicity, waste generation, and overall environmental impact. These results illustrate that sustainable synthetic practices can be successfully implemented without compromising reaction efficiency or educational value. Importantly, this work highlights the feasibility of integrating green chemistry principles—such as safer solvents, waste minimization, and improved atom economy—into undergraduate research and teaching laboratories.

Beyond the synthetic outcomes, this project serves as a model for incorporating green chemistry into undergraduate education through hands-on research. The approach reinforces core concepts in organic synthesis while fostering student awareness of sustainable laboratory practices. This study supports the broader adoption of green chemistry methodologies in academic settings and demonstrates their value in both research and pedagogy.

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EES - D3 - P02
CO_2 upcycling to liquefied petroleum gas and jet fuel via an oxide–zeolite catalyst strategy

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Sustainable aviation fuels (SAF) synthesized via Power-to-Liquids (PtL) processes utilizing CO_2 and green hydrogen represent a critical pathway for decarbonizing the aviation industry. However, synthesizing jet fuels through CO_2 hydrogenation presents challenges in overcoming the Anderson–Schulz–Flory distribution and optimizing the olefin-to-paraffin ratio to meet strict fuel specifications. This study proposes an oxide–zeolite (OXZEO) strategy to produce jet-range paraffins using a bifunctional catalytic system comprising an Fe-K supported copper aluminum spinel (FKC) oxide catalyst and a proton-form MFI zeolite. To enhance the diffusion of bulky $C_{8\text{-}16}$ hydrocarbons, a mesoporous nanosheet-type zeolite (NS) was introduced and loaded with Pt metal to facilitate olefin hydrogenation. In-situ DRIFTS analysis revealed that the NS catalyst with 1 wt% Pt exhibits superior hydrogen dissociation capabilities due to a high surface Pt^0 ratio. This functionality promotes formate formation in the FKC, shifting the thermodynamic equilibrium toward CO_2 consumption while simultaneously enhancing the hydrogenation of olefins. Consequently, this catalytic design achieved the highest paraffin ratio within the $C_{8\text{-}16}$ composition, demonstrating a practical approach for effective CO_2 upcycling into high-quality aviation fuel.

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2024-00466475 and RS-2024-00349276).

EES - D3 - P03
Understanding the effects of cryomilling for some common thermoplastics

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It has been known since the times of Staudinger[1] that mechanical force can break polymer chains by cleaving chemical bonds. This simple phenomenon can be used for beneficial purposes, such as in polymer recycling[2], mechanochemical copolymerization reactions, or other chemical reactions initiated by the generated mechanoradicals[3] (or to mitigate adverse effects like static charging caused by these radicals[4]). However, the vigorous, seemingly uncontrolled milling process does not provide the necessary 'fine' processing for these purposes. Yet, with global annual thermoplastic production of 445 million tons (290 billion dollars in value) and the growing need to reuse polymer materials, ball milling can be harnessed to deliver useful products.
This study involves cryomilling of some common polymers, polyethylene, polypropylene, polystyrene, poly(vinylchloride), and polyethylene terephthalate, which are the main players in the plastics market today. Cryomilling[5] must be used to avoid mastication of plastics and to increase bond-breaking efficiency. As the process itself also consumes energy and liquid nitrogen, polymers were milled for short durations (up to 10 minutes) to yield the desired structural and chemical changes in the selected polymers. Each milling parameter, such as jar material, milling frequency, and ball count, was evaluated for its effect on the overall bond-breaking process. In these analyses, the molecular weights of the polymers were monitored by gel permeation chromatography (GPC), oxidation of the milled material was tracked by X-ray photoelectron spectroscopy (XPS), and changes in crystallinity were determined by X-ray diffraction (XRD), along with other complementary characterization techniques. Quantitative analyses of the mechanoradicals formed during the milling were carried out by 2,2-diphenyl-1-picrylhydrazyl (DPPH) tests.[6] The results show that, depending on the chemical structure and crystallinity of the milled material, the milling outcome can be drastically different. Depending on the polymer structure, bond breakage can be heterolytic or homolytic, thereby diversifying the chemical species obtained.[7]

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EES - D3 - P04

Unraveling the electrocatalytic performances and structural stability of Ag nanowire gas diffusion electrodes for CO_2 reduction

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The electrochemical reduction of CO_2 (eCO_2RR) offers a sustainable route for converting CO_2 into more value-added products, with carbon monoxide being a key component of syngas and in other industrial processes.[1] Among the range of catalysts explored for the selective electrochemical reduction of CO_2 to CO, silver has received considerable attention. In particular, silver nanowires (AgNWs) are distinguished by their high electrical conductivity, tunable morphology, and large electrochemically active surface area.[2] In this work, AgNW gas diffusion electrodes (GDEs) synthesized from a modified polyol method, were evaluated for eCO_2RR under different reaction environments and cell configurations. Reasonable faradaic efficiency for CO, exceeding 90%, could be obtained at –1.7 and –1.8V vs Ag/AgCl in 3-electrode flow cell setup and at cell voltage between 2.8 and 3V in zero gap electrolyser setup with a catalyst load of 0.2 - 0.3 mg/cm^2. Long term electrolysis tests showed stable operation for approximately 8 hours, followed by a gradual decline in CO selectivity, primarily attributed to salt precipitation and pore blockage within the GDE and the flow channels. Variation of CO_2 flow regimes demonstrated that reduced gas flow enhanced overall CO_2 conversion efficiency, up to 34% at 3.5V, compared to 12% at higher flow rates. Post-electrolysis characterization of the AgNWs surface revealed partial removal of the polyvinylpyrrolidone (PVP) capping layer and important morphological alterations in the nanowire network, though the overall catalytic activity remained largely preserved.

Keywords: CO_2 reduction reaction, Ag nanowire, Gas diffusion electrodes, Conversion efficiency, Morphological instability

EES - D3 - P05
Pilot-scale online monitoring of CESAR1 solvent condition in a cement CO_2 capture plant

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Chemical CO_2 capture using amine-based solvents is a cornerstone technology for achieving deep decarbonization in hard-to-abate industrial sectors such as cement production[1]. Despite advances in solvent energy efficiency and degradation resistance, solvent degradation remains a major challenge for reliable long-term operation of industrial-scale capture plants, leading to solvent loss, corrosion, and increased operating costs. Now solvent condition is mainly assessed through periodic sampling and labour-intensive offline analyses, resulting in delayed feedback and limited ability to implement proactive mitigation strategies.
This work presents the development and pilot-scale deployment of an online monitoring approach based on liquid-phase Fourier Transform Infrared (FTIR) spectroscopy for continuous assessment of the CESAR1 solvent system. The study is conducted at a continuously operated CO_2 capture pilot plant at a cement production facility in Aalborg, Denmark. The installation has a capture capacity of approximately 1 ton CO_2 per day[2]. CESAR1, a blend of 2-amino-2-methyl-1-propanol (AMP) and piperazine (PZ), is monitored online, including AMP and PZ concentrations, CO_2 loading, and solvent degradation behaviour. An in situ FTIR probe installed directly in the solvent loop enables high-frequency spectral acquisition without sampling or process interruption (**Figure 1**).

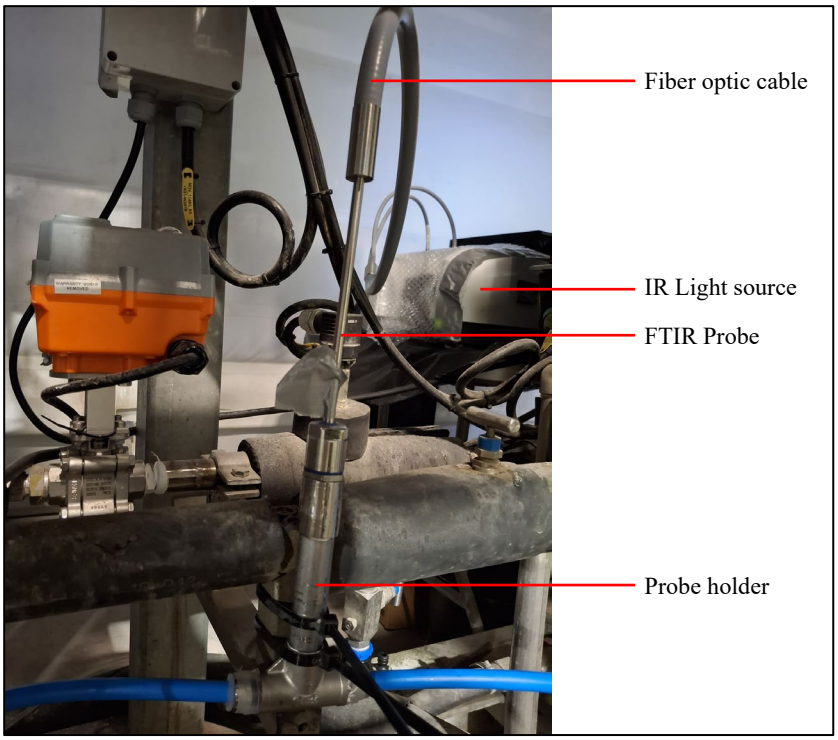

Fig. 1. In-situ FTIR probe connected to IR light source by a fibre optic cable

Quantitative interpretation of the FTIR data is done through offline reference analyses using ion chromatography, which are used to correlate characteristic spectral features with solvent composition, CO_2 loading, and degradation indicators. Machine learning models were trained and optimized using pilot plant data complemented by laboratory-prepared samples. Representative model validations for AMP and a characteristic degradation marker are shown in **Figure 2**, demonstrating agreement between predicted and measured concentrations across the observed operating range.

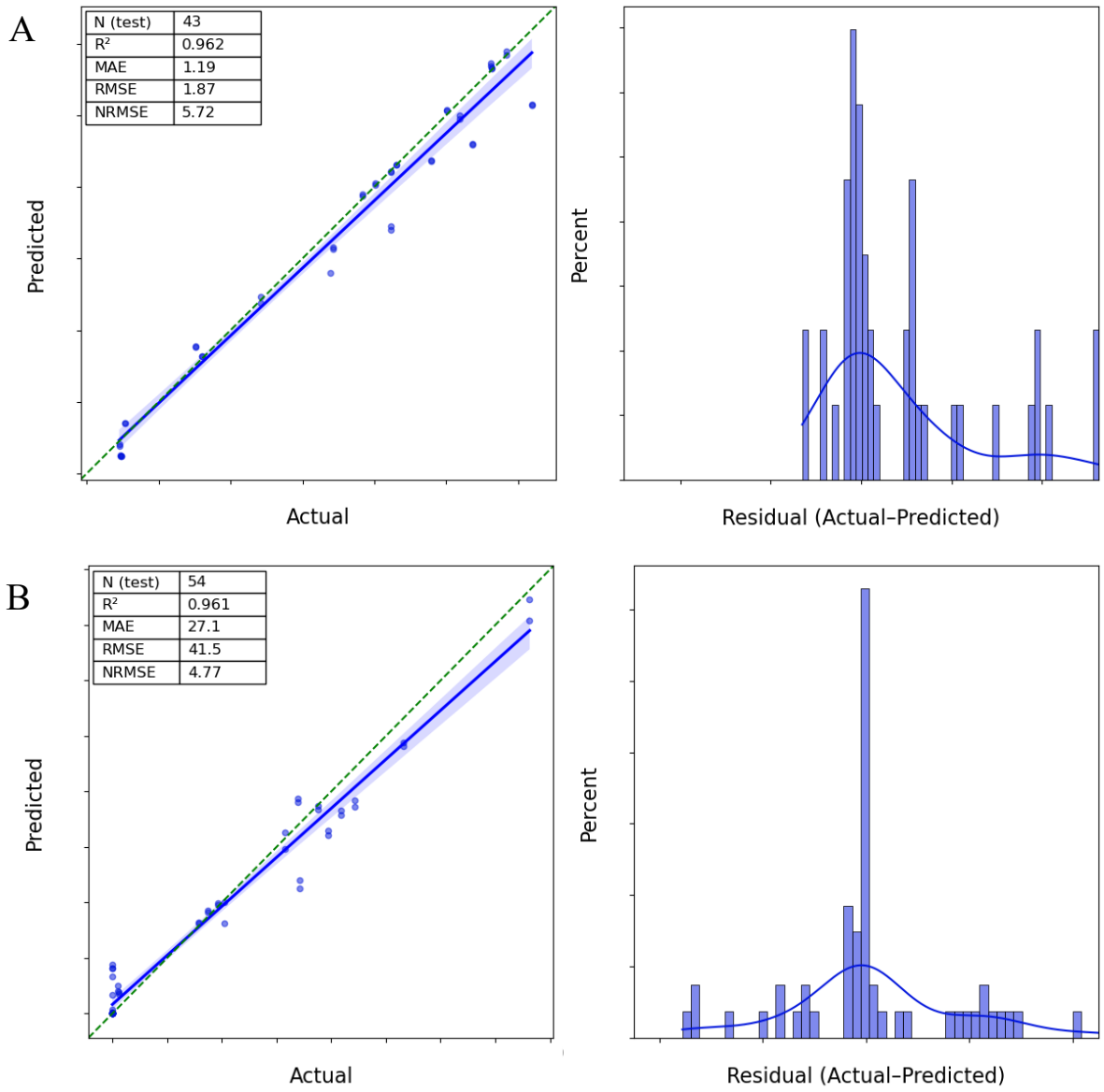

Fig. 2. A) Validation of a PLS model of AMP B) Validation of a PLS model of a specific solvent degradation marker

The continuous nature of the monitoring overcomes the limitations of periodic sampling, making it possible to detect degradation trends and support proactive operational strategies such as optimized solvent reclaiming and real-time evaluation of degradation inhibitors. Overall, the results demonstrate that in situ FTIR spectroscopy is a promising tool for online solvent monitoring in CO_2 capture applications.

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EES - D3 - P06

Sustainable integrated approach for CECs removal in aquaculture: Bench-scale validation of a hybrid membrane-AOP system

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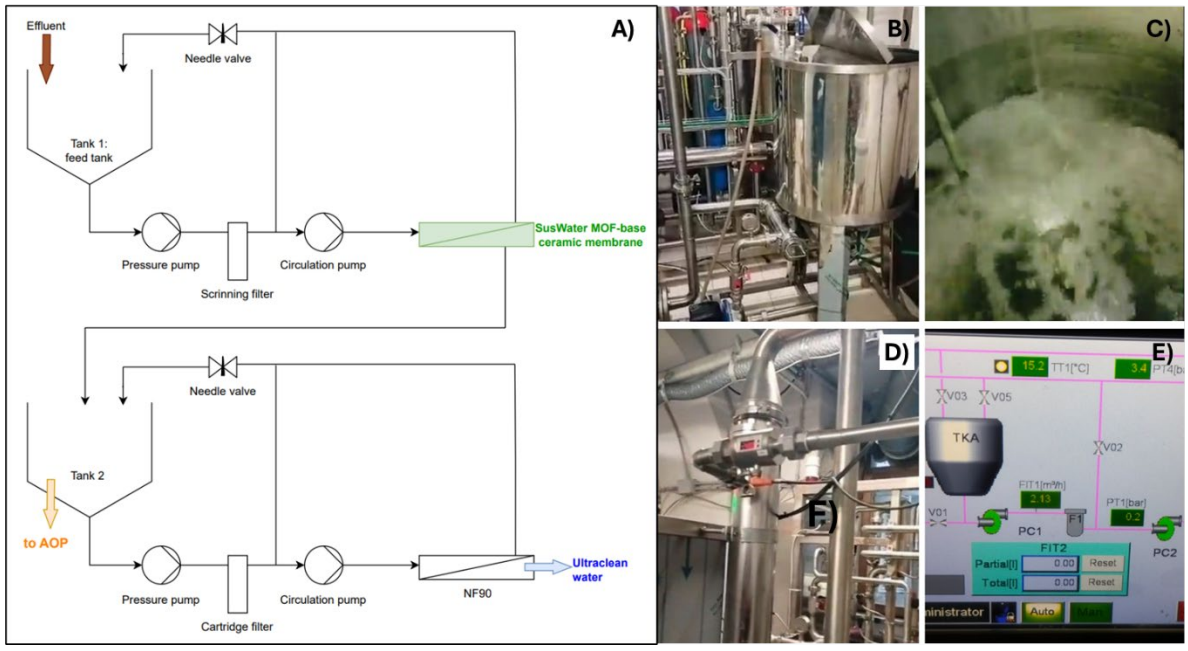
Aquaculture is a rapidly expanding sector demanding sustainable water management strategies to mitigate the release of contaminants. The feasibility of an integrated treatment sequence combining novel ceramic membranes and advanced oxidation processes (AOPs) for water reuse was explored. A nanostructured ceramic membrane coated with ZIF-8@ SiO_2-ZrO_2 gel core-shell nanoparticles was successfully upscaled from laboratory development to a real-scale multichannel module (1179 mm length, 25 mm diameter) and validated at bench scale using real aquaculture effluents spiked with sulfamethoxazole and carbamazepine as model micropollutants. The ceramic membrane exhibited high permeability, mechanical robustness, and chemical resistance, enabling direct treatment of fish farm effluents and effective protection of downstream technologies. While showing moderate selectivity toward micropollutants, the membrane proved to be well suited as a pretreatment step for nanofiltration. Integration with NF90 nanofiltration enabled efficient concentration of pollutants into the retentate, subsequently treated by photocatalysis using a co-doped P-In-C_3N_4 catalyst. The tailored co-doping enhanced charge separation and reactive species generation, enabling complete removal of contaminants under simulated solar irradiation despite the complex retentate matrix.
The innovation of the proposed approach lies in two complementary steps: first, the application of a MOF-based ceramic coating on a real-scale membrane module can be used as a unique pretreatment for complex aquaculture effluents, even under spiked conditions, prior to nanofiltration; second, the integration of photocatalysis directly addresses the issue of contaminant accumulation in the concentrated retentate, allowing efficient treatment of a reduced-volume stream that would otherwise be problematic for AOPs.



(A) Schematic representation of the bench-scale setup and pictures of (B) the feed tank, (C) the treated aquaculture water, (D) the membrane housing, and (E) the HDI to operate the system.

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EES - D3 - P07
Composition and efficacy of essential oils in suppressing potato sprouting

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University of Warmia and Mazury in Olsztyn, Poland

Potatoes are one of the most commonly consumed foods in the world, but their natural tendency to sprout during storage poses a significant technological problem. Extending the storage life of potatoes involves controlling temperature and using sprout inhibitors. One of the most commonly used compounds was chlorpropham (CIPC). However, growing concerns about its harmfulness have led to the withdrawal of CIPC in the European Union (EU) and the search for alternative solutions. The most interesting alternatives are natural essential oils (EOs)[1]. The EO best described in the scientific literature is caraway EO, which contains carvone. Biopreparations containing carvone based on spearmint EO are already approved for marketing in the EU.
In our studies, we have shown that other EOs have a suppressive effect on potato sprouts, including coriander seeds (*Coriandrum sativum* L.), dill seeds (*Anethum graveolens* L.), tansy (*Tanacetum vulgare* L.) and thuja (*Thuja occidentalis* L.). EOs were produced by hydrodistillation in a Deryng apparatus (10 dm^3). The chemical composition of EOs was determined by GC-MS using a Schimadzu QP-2020NX system. A correlation was found between the content of carvone, phellandrene, thujone and the bioactivity of EOs. However, a question to be addressed in future studies will be to determine the safety of using EOs containing harmful thujone (thuja, tansy). EOs from dill and coriander are safer, as is caraway oil.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P08

Comparison of the yield and chemical composition of essential oils from the seeds, leaves and straw of *Apiaceae* plants

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Essential oils (EOs) are products derived from plant raw materials, obtained by steam distillation, hydrodistillation, and less frequently by pressing and dry distillation. EOs generally consist of mixtures of terpenoids, phenylpropanoids, esters, aldehydes, and alcohols. The components of EOs are very interesting from an application point of view. EOs have unique properties (volatility, pleasant smell, bioactivity), which make them widely used in industry, medicine and agriculture[1,2].

The aim of the study was to compare the chemical composition of EOs produced from different parts of plants (seeds, leaves and waste straw) of species from the *Apiaceae* family: dill, fennel, caraway, coriander, celery, parsley. EOs were produced by hydrodistillation in Deryng apparatus (10 dm^3). The chemical profile of EOs was determined by GC-MS using a Schimadzu QP-2020NX system. The results of our study revealed that the highest EO yield was obtained from seeds, especially caraway (2.66% v/m) and dill (1.90%). In the case of EOs from leaves, celery had the highest yield (0.26%). This is important because celery leaves are often a by-product of horticulture. Dill straw contained the least amount of EO (only 0.10%). *Apiaceae* EOs were characterised by a diverse chemical composition. For example, the dominant components of dill EO were α-phellandrene, β-cymene and D-limonene, while caraway EO contained D-carvone and D-limonene. The straw, leaves and seeds of a given species had a similar EO chemical profile.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P09
Contact electrification of some organic powders with fused aromatic ring structures

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Static charge accumulation on insulating surfaces causes a variety of issues in many industries. The mechanism of charge accumulation via contact and subsequent charge dissipation has been studied since ancient times, yet it remains poorly understood. The static charge-related problems are even more pronounced when powder materials are involved.
In this study, our objective is to provide a more systematic perspective on the charging of organic material powders. The basic question is whether the chemical structure is a dominant factor in the triboelectrification of insulating powders. Therefore, simple and common aromatic powders with varying numbers of aromatic rings are analyzed according to their charging propensities under identical conditions. Also, we studied the impact of the type, number, and position of certain functional groups in the molecular structure on the material's triboelectrification.
We ground the powder materials in an agate mortar with a steel and agate pestle to charge them. An electrostatic voltmeter was then used to measure the electric potential developed on the powder. The results show sign and magnitude of the electrostatic potential seemed to be related to the number of fused aromatic rings. Additionally, powders of some compounds bearing functional groups, such as nitro or carboxyl, were negatively charged, while powders with molecular structures bearing a methyl group were positively charged. We studied particle morphology via SEM and crystallinity via XRD analysis to determine whether these material attributes change before and after grinding and whether these changes make a decisive contribution to the electrification outcome. Our results show that, as hypothesized, the molecular structure is the largest influencer of powder triboelectrification. We believe that a fundamental understanding of the physical properties and chemical structure can help solve future powder charging-related problems.

EES - D3 - P10

Directional charge transport in donor–acceptor covalent organic frameworks for enhanced photocatalytic H_2O_2 production

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The development of efficient photocatalysts requires the optimization of several interrelated factors, including light absorption, exciton generation and dissociation, charge transport, band alignment with redox reactions, and surface properties. Donor–acceptor (D–A) two-dimensional covalent organic frameworks (COFs) are promising photocatalysts due to their ability to facilitate exciton separation. However, the preferred direction of charge transport (whether within the plane or along the out-of-plane (z) direction) and its role in catalytic performance remain unclear. Here, we examine charge-transfer pathways in three structurally comparable D–A COFs (TAPD–TT, TAPD–TFTA, and TAPD–TA) constructed from the electron-rich knot N,N,N′,N′-tetrakis(4-aminophenyl)-1,4-phenylenediamine (TAPD) and acceptor linkers with systematically varied electron densities. Using a combination of experimental techniques and density functional theory (DFT), we correlate photophysical behavior with photocatalytic H_2O_2 production.

Exciton separation occurs predominantly within the two-dimensional planes through the D–A effect, with comparable separation efficiencies across all three COFs, indicating that pronounced donor–acceptor electron density differences are not strictly required. Hole transport is efficient in all directions, showing a clear preference for in-plane motion with effective masses between 0.5 and 1.4 m_e. In contrast, electrons are heavy in the xy-plane, with effective masses near 6 m_e. Along the z-direction, however, TAPD–TT exhibits a substantially lower electron effective mass (~2.5 m_e), markedly smaller than those of TAPD–TFTA and TAPD–TA. This enhanced out-of-plane transport in TAPD–TT arises from tight vertical stacking of TT acceptor units, which maximizes π–π overlap and enables efficient interlayer electron mobility. The resulting directional charge transport directly correlates with superior photocurrent generation and the highest H_2O_2 production rate.

These findings establish structure–charge transport–activity relationships and highlight directional electron mobility as a decisive design parameter for high-performance photocatalytic COFs.

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EES - D3 - P11
Inhibition of seed germination by selected essential oils: Relationship with chemical composition

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Essential oils (EOs) are volatile liquid substances obtained from plant materials through steam distillation. In recent years, EOs have been the subject of interest as potential bioherbicides, which is in line with the idea of bioeconomy and green chemistry[1]. The aim of this study was to determine the chemical composition of EOs obtained from selected plant materials and to evaluate their inhibitory effect on seed germination (phytotoxicity). The research material consisted of: (1) herbs: tansy (*Tanacetum vulgare* L.), Canadian goldenrod (*Solidago canadensis* L.); (2) seeds: dill (*Anethum graveolens* L.), caraway (*Carum carvi* L.), coriander (*Coriandrum sativum* L.); (3) biomass of whole plants: Scots pine (*Pinus sylvestris* L.), thuja (*Thuja occidentalis* L.), Nordmann fir (*Abies nordmanniana* (Steven) Spach). Essential oils were obtained by hydrodistillation in a Deryng apparatus (10 dm^3). The chemical profile was determined by GC-MS using a Schimadzu QP-2020NX system. Biological activity was determined in phytotoxicity tests. The tested EOs were characterized by a very complex chemical composition. Each of them contained at least several dozen volatile organic compounds, and the longer the hydrodistillation was carried out, the higher the number of detected compounds and their molecular weights. The main components were monoterpenoids and sesquiterpenoids. It was shown that most of the tested EOs exhibit allelopathic activity. Some of them can potentially be used as bioherbicides, especially those from thuja, coriander, dill, and tansy.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P12

Predictive chemometric modeling of molecular transport in functional organic solvent nanofiltration membranes

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Organic solvent nanofiltration (OSN) membranes have widespread industrial applications. In this study, ensemble machine learning (ML) coupled with chemometric modeling was applied to functionalized polyacrylonitrile (PAN)–supported poly(piperazine-amide) thin-film composite (TFC) membranes to enable data-driven prediction of OSN performance. Diamines such as ethylenediamine (EDA) and hydrazine (Hz) were cross-linked with PAN membranes to produce functionalized supports, and their impact on TFC membrane performance for OSN was systematically investigated. Membrane characterization confirmed that diamine functionalization enhanced poly(piperazine-amide) formation, as evidenced by ATR-FTIR and surface charge analyses. The EDA-cross-linked PAN-supported TFC membrane exhibited minimal solvent swelling, while the hydrazine-modified TFC membrane displayed pronounced hydrophilic characteristics. EDA-TFC and Hz-TFC membranes enhanced polar and aromatic solvent transport through specific hydrogen-bonding, dipolar, and π–π interactions governed by solvent solubility, viscosity, and molecular size. Dye separation experiments using Rose Bengal (RB), Congo Red (CR), Eriochrome Black T (EBT), and Methylene Blue (MB) confirmed that solvent transport and selectivity are strongly influenced by diamine-modified PAN–TFC support chemistry. The EDA-TFC membrane achieved the best balance between flux and rejection, whereas the Hz-TFC membrane delivered higher organophilic flux but with reduced selectivity toward cationic dyes. Accurate prediction of solute transport in OSN is essential for industrial scale-up due to complex solvent and solute–membrane interactions. However, the Spiegler–Kedem framework, while mechanistically informative, is limited by its reliance on constant transport parameters across diverse systems. Principal component analysis (PCA) revealed clear grouping of transport- and interaction-related descriptors, with solvent affinity dominating PC1 and steric and surface effects (molecular size, CN-index, contact angle) defining PC2, in agreement with correlation trends. Among Gaussian process regression (GPR) models, the comprehensive C1 descriptor set delivered near-perfect predictive accuracy (R2 test = 0.986, RMSE test = 0.703)., outperforming reduced descriptor by effectively capturing coupled transport, steric, and surface-chemistry effects governing dye rejection.

Keywords: Gaussian process regression; Machine learning; Organic solvent nanofiltration (OSN); Thin-film composite (TFC).

EES - D3 - P13

Sunlight-powered reverse water gas shift reaction catalysed by plasmonic Au/CeO_{2-x}: The impact of size, metal loading and oxygen vacancies on the catalytic performance

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The reverse water gas shift (rWGS, eq. 1) reaction is an attractive pathway for CO_2-to-CO conversion; however, it is endothermic and directly competes with the exothermic Sabatier methanation reaction (eq. 2), requiring high temperatures for CO selectivity. Photocatalysis offers a low-temperature alternative.[1,2]

rWGS $\quad CO_2 + H_2 \leftrightarrows CO + H_2O \quad \Delta H_{298K} = +41.2\ \text{kJ mol}^{-1}$ (1)

Sabatier reaction $\quad CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \Delta H_{298K} = -165.0\ \text{kJ mol}^{-1}$ (2)

In this study, we selected Au/CeO_{2-x} as plasmonic catalyst for the sunlight-powered rWGS reaction. A systematic study of the impact of Au particle size and loading on the its catalytic performance has not yet been reported. Furthermore, the influence of oxygen vacancies is unknown. We focus on elucidating the impact of these characteristics on the catalytic performance.

We successfully produced Au/CeO_{2-x} catalysts.[3] Both size of Au and CeO_{2-x} was varied and the Au loading on the CeO_{2-x} surface (Fig. 1). Furthermore, various techniques were applied to tailor the concentration of oxygen vacancies.

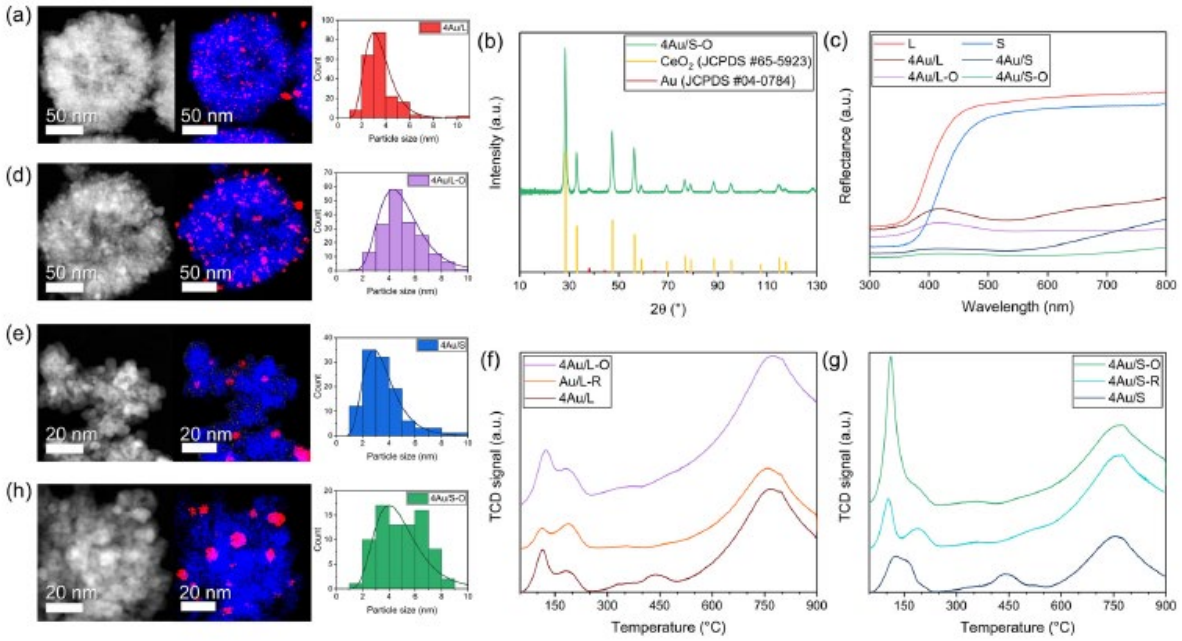

Fig. 1. Representative HAADF-STEM image, EDX mapping in STEM mode and Au particle size distribution from TEM analysis with lognormal fit of various Au/CeO_{2-x} catalysts (a, d, e, h). CeO_{2-x} is coloured blue and Au is coloured red in EDX mapping, lower magnification shown for (a) and (d) to illustrate CeO_{2-x} size particle difference. (b) XRD diffractogram of 4Au/S-O. (c) Reflective diffuse UV-vis spectra of various (Au/)CeO_{2-x} catalysts; graphs have been stacked for visual clarity. H_2-TPR profiles of (f, g) various Au/CeO_{2-x} catalysts; graphs have been stacked for visual clarity.[3]

By assessing the performance of the catalysts, we obtained following key findings: (1) Upon illumination, all catalysts produced CO with a selectivity of ≥98% at low catalyst surface temperatures; (2) The CO production rate increased exponentially with the irradiance, confirming photothermal heating; (3) In dark, all catalysts formed CH_4

instead of CO, indicating that plasmon-induced desorption of CO plays a vital role; (4) The activity depends linearly on the accessible interfacial area between CeO_{2-x} and Au, which is in line with an associative reaction mechanism.[4] Currently, we are focusing on preparing catalysts with a high loading of small Au nanoparticles to study the impact of interparticle distance. To achieve high loadings of small Au nanoparticles, we designed a new Au deposition step involving Sn-mediated nucleation. To date, we have successfully prepared Au/CeO_{2-x} catalysts using this technique (Fig. 2). We are currently optimizing this synthesis procedure and assessing the performance of these catalysts.

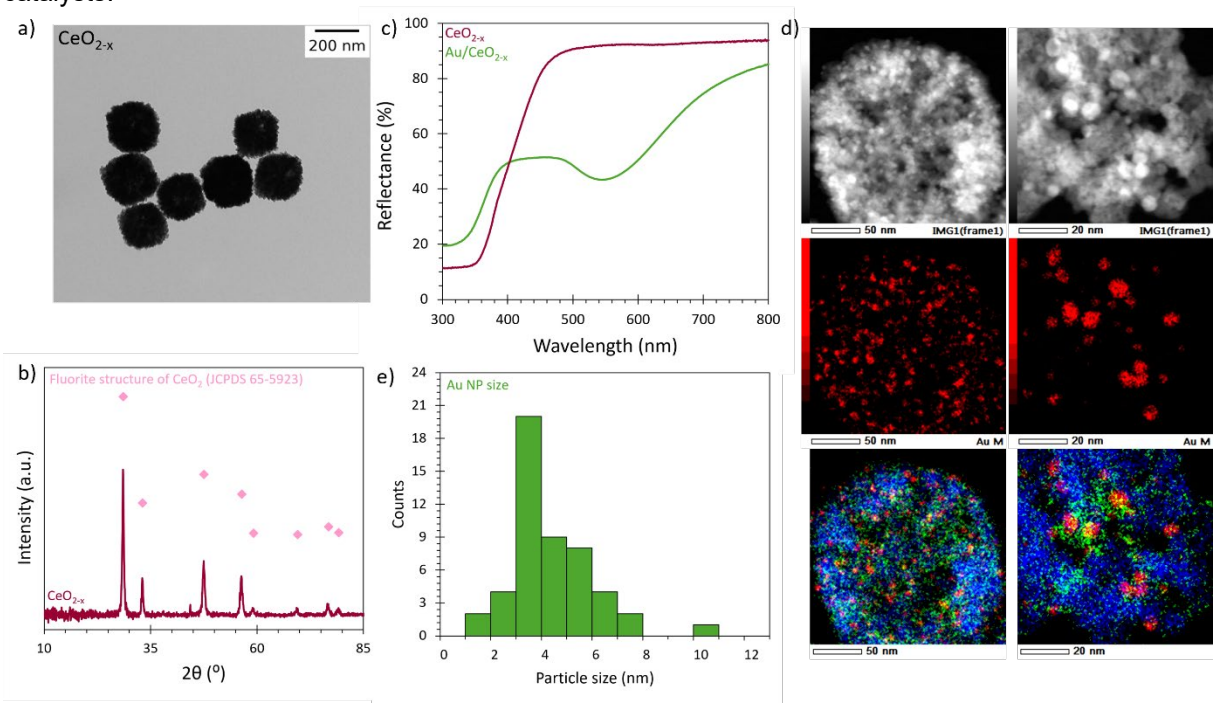

Fig. 2. (a) TEM image of CeO_{2-x} particles, with an average particle radius of 121.1 ± 1.13 nm calculated from multiple images. (b) XRD diffractogram of CeO_{2-x}; the crystallite size, calculated using the Scherrer equation from the (111) diffraction peak at $2\theta \approx 28.5°$, is 19.75 ± 1.72 nm. (c) Diffuse-reflectance UV-Vis spectra of CeO_{2-x} and Au/CeO_{2-x}. (d) Representative HAADF-STEM image and corresponding STEM-EDX elemental maps of Au/CeO_{2-x} with a theoretical gold loading of 5.5 wt%, showing Ce in blue, Sn in green, and Au in red. (e) Histogram of the gold nanoparticle size distribution for Au on CeO_{2-x}, determined from STEM-EDX analysis, with an average particle size of 4.38 ± 1.69 nm.

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EES - D3 - P14
Safe and sustainable materials as adsorbents for emerging pollutants

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The increasing demand of polymeric materials in combination to the interest in preventing environmental pollution recently brought to the design and synthesis of polymeric materials from sustainable feedstocks. Several efforts have been devoted to the synthesis of bio-based polymers via ring-opening metathesis polymerization from epoxidized soybean oil and its copolymerization.[1,2] While the polymerization of the crude soybean oil is less investigated, in this framework an easy conversion of soybean oil in a durable and chemical degradable material has been recently reported.[3]
The bio-polymer can be efficiently applied for wastewater pollutant removal such as dyes, oil and halogenated solvents. However, since December 2024, wastewater treatment has been subject to new regulations (namely, Directive EU. 3019/2024), prompted by the systematic detection of emerging pollutants (microplastics, perfluoroalkyl substances (PFAS), pharmaceutically active compounds (PhACs)). For this reason, the research of new materials able to trap emerging pollutants is urgent.
In this framework, the soybean-oil-derived bio-based polymer mixed with zeolite was evaluated also as a sustainable adsorbent for the removal of an antibiotic, such as doxycycline (DOX), from treated wastewater. Batch tests with a 50:50 mixture of biopolymer and zeolite at initial DOX concentrations of 2.5–7.5 mg L^{-1} achieved 50–60% removal at 2.5–5 mg L^{-1} and nearly complete (≈99%) removal at 7.5 mg L^{-1} after 48 h. Pilot columns packed with the same material treated 100 L of spiked tertiary effluent (1 L h^{-1} for 4 days), exhibiting S-shaped breakthrough curves and sustained antibiotic retention under realistic hydraulic conditions, with faster exhaustion at higher influent loads. Regeneration tests identified 2-methyl-tetrahydrofuran as the most effective solvent for DOX desorption that allows the recyclability of the adsorbent for further adsorption cycles. The results demonstrate the technical feasibility of this regenerable, bio-based material as a candidate adsorbent for conventional and quaternary treatment of urban wastewater.

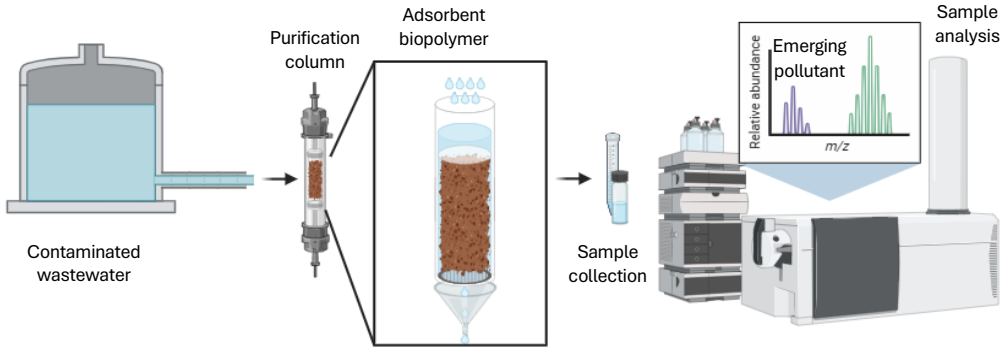

Fig.1. Schematic representation of the pilot scale experimental set-up in which the biopolymer is used as adsorbent material.

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EES - D3 - P15
Understanding structural and electrochemical degradation in Li-rich cathodes

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Li-rich layered oxides (LRLOs) are promising high-capacity cathode materials for lithium-ion batteries, offering capacities above 200 mAh g^{-1} through combined cationic and anionic redox activity [1]. Their application is limited by structural and electrochemical instabilities, including transition metal redistribution, microstructural damage, and voltage decay [2]. In this study, a Co-free LRLO with composition $Li_{1.18}Mn_{0.52}Ni_{0.3}O_2$ was synthesized via a solid-state route combining ball milling and calcination and tested in lithium cells using both a conventional carbonate-based electrolyte and an ionic liquid-based electrolyte. Ex situ synchrotron X-ray fluorescence (XRF) 2D imaging at multiple length scales was employed to probe the spatial distribution of transition metals within electrode particles. The measurements show that cycling in the carbonate-based electrolyte induces manganese redistribution and localized heterogeneities, associated with early microstructural changes [3], whereas the ionic liquid electrolyte preserves a more uniform distribution of transition metals and a more intact electrode structure. These findings indicate that manganese migration contributes significantly to the structural and electrochemical degradation of Co-free LRLOs and that electrolyte composition can influence the extent of these effects. By linking transition metal distribution to cycling behavior, this study provides direct experimental insight into degradation mechanisms in Li-rich cathodes, supporting the development of strategies to improve their stability and lifetime.

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EES - D3 - P16
Controlled incorporation of monoboc-protected amines in polyamide thin-film composite membranes

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Thin-film composite polyamide membranes were fabricated via interfacial polymerization with controlled incorporation of ethylenediamine monoboc (EDAM) as a functional amine modifier. By varying the proportion of EDAM during membrane formation, a series of chemically tailored membranes with distinct structural and surface characteristics were obtained. The membranes were systematically characterized using spectroscopic, microscopic, thermal, and surface analyses to confirm successful modification and to evaluate changes in morphology, chemical composition, wettability, and stability. The influence of amine modulation on membrane transport behavior was further examined under pressure-driven filtration conditions. This study demonstrates a versatile strategy for fine-tuning polyamide membrane properties through controlled amine chemistry, offering a scalable route toward next-generation membranes with improved performance and tunable physicochemical features for water and separation applications.

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EES - D3 - P17
Recovery and regeneration of cathode materials via direct recycling

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The rapid expansion of electric vehicles and portable electronics is driving a sharp increase in lithium-ion battery production, intensifying pressure on critical raw materials (CRMs) and resulting in a growing volume of end-of-life batteries that still contain significant amounts of valuable metals[1]. Developing sustainable recycling strategies capable of closing the loop is therefore a key challenge for the battery value chain.
Direct recycling has gained increasing attention as it aims to recover cathode materials while preserving their original structure and functionality. By avoiding complete elemental breakdown, this strategy has the potential to reduce energy consumption and environmental impact compared to conventional recycling routes.
Here, we investigate the recovery and regeneration of NMC materials from spent lithium-ion cells. Different routes were explored to separate the active material from the current collector, including mechanical and solvent-based delamination methods. All approaches enabled effective recovery of the cathode powder, although typical degradation and processing related impurities were observed in the recovered material. Regeneration of the spent cathode was carried out through solid-state relithiation designed to restore stoichiometry and structural order. Chemical-physical characterization confirmed the re-establishment of the layered structure while the electrochemical characterization demonstrated that the regenerated material recovered a substantial fraction of its original performance.
Overall, this study demonstrates the effectiveness of direct recycling for regenerating cathode materials from end-of-life LIBs[2]. The results highlight the potential of this approach to support a more circular battery economy by reducing waste, lowering environmental impact, and decreasing dependence on critical raw material supply.

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EES - D3 - P18

Advanced sorption-based recovery of rare-earth elements from secondary aqueous streams: A contribution to EU strategic autonomy and circular critical raw materials

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The accelerating deployment of low-carbon and digital technologies has driven unprecedented demand for rare-earth elements(REEs), exposing the European Union's reliance on imports and primary mining, mainly outside Europe. This reliance poses risks to supply security and sustainability. In alignment with the EU Critical Raw Materials Act, EU Green Deal, and Horizon Europe strategic autonomy goals, efficient recovery of REEs from secondary sources is essential to foster circular critical raw material value chains and reduce environmental burdens[1,2].

Here we investigate a microporous niobium–iron silicate ($Na_{2.9}(Nb_{1.55}Fe_{0.45})_2Si_2O_{10}\cdot xH_2O$) as a sorbent for REEs removal from complex aqueous matrices, including spiked mineral water and simulated electronic waste leachates from permanent magnets and phosphors. Using Response Surface Methodology to optimise pH, initial REE concentration, and sorbent dosage, we demonstrate effective removal across realistic conditions.

Under optimised conditions (pH 4; 180 mg/L sorbent; 2 µmol/L REEs), removal efficiencies exceeded 80% for neodymium (Nd) and 60% for yttrium (Y) in mineral water within 6h. In e-waste solutions, both Nd and Y were removed at >95% efficiency at 5–10 µmol/L. Kinetic modelling indicates chemisorption-dominated uptake, with distinct behaviours consistent with heterogeneous sorption sites and ion-exchange processes.

These results position this sorbent as promising candidates for scalable, non-extractive REE recovery from secondary aqueous streams, advancing EU objectives to strengthen critical raw material resilience and sustainability[2,3].

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EES - D3 - P19
Chemical compositions, stability and insecticidal activities of some essential oil emulsions

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Essential oils (EOs) generally consist of mixtures of terpenoids, phenylpropanoids, and other classes of volatile organic compounds. These compounds are very interesting from a scientific and application point of view. For this reason, they are used in the production of flavors, perfumes, cosmetics, repellents, and even medicines and biopesticides[1]. Currently, biopesticides based on EOs from orange, spearmint, and tea tree are already registered on the EU pesticide market.
The aim of our research was to investigate the chemical composition, stability, and insecticidal activity of oil/water emulsions produced from EOs. EOs were produced from the seeds of *Apiaceae* plants: dill (*Anethum graveolens* L.), fennel (*Foeniculum vulgare* Mill.), caraway (*Carum carvi* L.), coriander (*Coriandrum sativum* L.) and biomass from selected coniferous trees. The emulsions were produced from EOs, surfactants (Tween, saponin) and water. The chemical composition of EOs and emulsions was determined using GC-MS. The stability of emulsions was assessed using the turbidimetric method. Insecticidal activity was determined in toxicity tests using *Tenebrio molitor* L. larvae. Based on the tests, it was shown that monoterpenes were the dominant compounds in EOs. Emulsions with EOs from *Apiaceae* seeds showed the best insecticidal efficacy (contact action). The respiratory action of EOs varied, with coriander EO showing the best efficacy. The results of our research show that EOs can be a source of promising bioactive compounds for the production of bioinsecticides.

Funding: The project entitled ‘Chemical composition and use of essential oils in the bioeconomy – development of the competences and skills of members of the Student Chemistry Research Club’ was co-funded by the European Union under the European Funds for Social Development Programme (FERS 2021-2027) and by the State budget (Poland) (agreement no. MNiSW/2025/DPI/592).

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EES - D3 - P20
Gold “self-leaching” in chloride-rich media

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In a technology-driven society, the demand for gold has increased due to its widespread use in advanced technologies. However, increased consumption has raised environmental concerns related to extraction and refining. Conventional methods rely on cyanidation, the dominant hydrometallurgical method, because of its efficiency and selectivity, but its extreme toxicity and long-term persistence present major regulatory challenges. These issues have motivated the development of safer, cyanide-free leaching technologies. Chloride-based leaching systems have emerged as promising alternatives, offering faster dissolution kinetics and improved environmental performance.
In the past few years, unconventional solvents such as ionic liquids and deep eutectic solvents (DES) have been gaining increasing attention in this regard because of their potentially minor environmental impact. Recent work in our laboratory[1] revealed a novel and fundamentally different leaching pathway for gold in the choline chloride-oxalic acid dihydrate (DES) through a comproportionation-driven reaction as shown below, which eliminates the need for external oxidants.

$$AuCl_4^- + 2Au + 2Cl^- \rightleftharpoons 3AuCl_2^-$$

This work demonstrates that the comproportionation reaction can occur in a wide range of chloride-rich systems, including aqueous and non-aqueous solutions, DESs, and ionic liquids, highlighting its versatility. Electrochemical and spectroscopic methods were employed to understand the leaching mechanism and to study the influence of acidity, chloride activity, and solvent viscosity on gold dissolution behaviour. The electrochemical data reveal that gold leaching proceeds under sustained non-equilibrium conditions and is strongly governed by mass-transport limitations rather than by thermodynamic equilibrium[2].
This mechanism enables efficient gold recovery with strong green credentials, highlighting its potential as a sustainable and environmentally benign alternative to conventional cyanide-based gold leaching.

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[2]F. Soma, O.Djorf, M.Bougouma, E.Muragijimana, T.Doneux. Gold “self-leaching“in chloride-rich media. *Submitted*.

EES - D3 - P21
High-temperature operation of vacuum tube solar collectors using Ionic liquids

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In recent decades, renewable energies have expanded worldwide to replace fossil fuels and mitigate climate change. The European Green Deal has accelerated this transition. Spain's favorable climate makes it ideal for solar technologies, particularly efficient vacuum tube solar thermal collectors operating at high temperatures [1].
This study evaluates the feasibility of replacing water, the conventional heat transfer fluid, with the ionic liquid 1-ethyl-3-methylimidazolium acetate as the working fluid in a vacuum tube solar collector. The primary motivation is to overcome the temperature limitation imposed by the phase change of water at 100 °C, since ionic liquids exhibit negligible vapor pressure and much higher thermal stability, enabling operation in the liquid phase at temperatures well above this threshold.
Experimental tests were carried out under full solar radiation conditions using an evacuated tube collector located at the University of Murcia. The system was first characterized using water and subsequently operated with the ionic liquid, maintaining equivalent operating conditions and several constant flow rates to ensure a reliable comparison. The results demonstrate that the ionic liquid allows outlet temperatures exceeding 120 °C without phase change, whereas water is limited to approximately 90 °C. At low flow rates (1 L min^{-1}), the ionic liquid exhibited significantly higher thermal and exergy performance, reaching exergy values close to 27 kW, compared with about 18 kW for water under optimal conditions.
The lower specific heat, high thermal stability, and extremely low vapor pressure of the ionic liquid result in larger temperature rises and safer operation at elevated temperatures. Overall, the findings confirm that ionic liquids constitute a technically viable and highly promising alternative heat transfer medium for solar thermal systems, particularly for industrial applications requiring high-temperature heat in the liquid phase.

a)

b)

Variable	Water	Ionic liquid
Outlet temperature	>90ºC	>120ºC
Temperature difference in collector	5-25ºC	Up to 70ºC
Useful heat adsorbed	18 kW	27 kW
Maximum thermal efficiency	80%	100%
Operation at T>100ºC	No, undergoes phase change	Yes, remains in liquid phase
Influence of flow rate	Efficiency decrease at high flow rates	Good efficiency at low flow rates
Thermal stability	Up to 100ºC	High thermal stability
Operational safety	Risk of overpressure	Safe
Economic viability	Economical and widely available	High cost

Fig. 3. a) Schematic of vacuum tube solar collector used in the experiments. b) Comparison of water and ionic liquid as thermal solar fluids.

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EES - D3 - P22

Synthesis-route effects on competing phase formation in $Na_{0.67}Mn_{0.75}Ni_{0.25}O_2$

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Layered transition metal oxides (LTMOs) are among the most promising cathode materials for sodium-ion batteries, yet their electrochemical performance is strongly influenced by phase competition arising from synthesis conditions.[1-2] In this work, we investigate the effect of synthesis route on the structural evolution and electrochemical behavior of $Na_{0.67}Mn_{0.75}Ni_{0.25}O_2$ prepared via solid-state (SS) reaction and sol-gel (SG) methods. Although both routes target the same nominal stoichiometry, they lead to distinct crystallographic outcomes: the SS route predominantly stabilizes the P2 phase, whereas the SG route favors the formation of a P3 phase. Comprehensive characterization using X-ray diffraction, XANES, EXAFS, scanning electron microscopy, and thermogravimetric differential scanning calorimetry reveals comparable bulk local structures but marked differences in morphology, surface chemistry, and crystallization pathways. Electrochemical testing demonstrates that the P2-SS material exhibits superior cycling stability and rate capability, while the P3-SG sample suffers from rapid capacity fading, attributed to structural rearrangements during repeated sodium insertion/extraction. Thermal analysis further highlights the role of synthesis kinetics in directing phase formation and stability. These results underscore that synthesis methodology, beyond nominal composition, plays a decisive role in determining phase stability and electrochemical performance in sodium layered oxides. Our findings emphasize the necessity of precise control over synthesis parameters to optimize Na-LTMO cathodes for high-performance sodium-ion battery.

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EES - D3 - P23
Matrix dependent photochemical transformation of sulfamethoxazole in natural and managed waters

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The photochemical fate of antibiotics in surface waters is strongly influenced by water matrix composition. Sulfamethoxazole (SMZ) is a widely used antibiotic and is frequently detected in aquatic environments, where its persistence and transformation products may pose ecological risks. In this study, we investigate how variations in water composition influence the degradation and persistence of SMZ under environmentally relevant sunlight conditions.
Photodegradation experiments were conducted in real water matrices collected from diverse geographical and environmental settings. Irradiations were performed using a solar simulator, so enabling the assessment of SMZ transformation under conditions dominated by matrix mediated photochemical processes rather than by direct photolysis of the compound.
Marked differences in SMZ degradation kinetics were observed among the water matrices investigated.
Slower transformation occurred in waters with low dissolved organic carbon (DOC), whereas significantly faster degradation was observed in humic-rich waters with high DOC content. These differences were attributed to matrix composition, particularly DOC concentration and fluorescence characteristics, which influence the formation and reactivity of photochemically produced reactive species. Probe compound experiments and oxygen-controlled irradiations indicate that triplet excited states of dissolved organic matter (^{3}CDOM*) play a key role in SMZ degradation in humic-rich matrices. Matrix-dependent transformation pathways led to the formation of distinct transformation products, including the selective production of a phenolic derivative in humic-rich waters, which is predicted to be more toxic than the parent compound. Overall, this study demonstrates that the environmental fate and risk profile of SMZ cannot be generalized, as they depend critically on sunlight exposure and, in particular, on the chemical composition of the receiving water body.

Acknowledgements: This research was funded by the European Union under the Marie Skłodowska Curie Actions (MSCA) Doctoral Network IN2AQUAS (grant agreement No 101119555) and by Research and Innovation Staff Exchange Suswater (grant agreement No 101007578).

EES - D3 - P24
Deep eutectic solvents-enabled closed and open-loop wastes battery recycling

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[1]University of Turin, Italy; [2]Sapienza, University of Rome, Italy; [3]Institute of Science, Technology and Sustainability for Ceramics (ISSMC-CNR), Italy; [4]URT_CAMPUS, Dept. of Chemical Sciences and Materials Technologies, CNR, Italy; [5]University of Milan Bicocca, Italy; [6]INSTM - National Inter-University Consortium for Materials Science and Technology, Florence, Italy

Current patterns of energy consumption are closely linked to global warming and climate change. The push toward climate neutrality by 2050 and the transition to a sustainable society depend heavily on harnessing renewable energy, which highlights the pivotal role of batteries in the EU's Green Revolution. In particular, lithium-ion batteries have driven the electronics boom. However, the EU lacks a dependable domestic battery supply chain, with raw materials and production facilities largely located abroad, underscoring the strategic need for recycling to build an alternative, more autonomous supply network. Existing recycling methods fall short on sustainability as they require very high temperatures or toxic solvents and involve energy-intensive steps to recover battery-grade materials.
Here, we create a sustainable recycling route (Figure 1) based on Deep Eutectic Solvents (DES), rethinking the entire supply chain, by a single-stage, energy-efficient regeneration of lithium cobalt oxide (LCO) battery cathodes [1]. In case where battery-grade materials cannot be recovered (e.g. lithium manganese oxide. LMO), we expand the scope toward the production of catalysts for biodiesel synthesis [2].
These innovative approaches promise an almost zero-waste, energy-saving recovery process for battery waste, helping to establish a resilient EU supply chain and positioning the Union at the vanguard of the green transition.

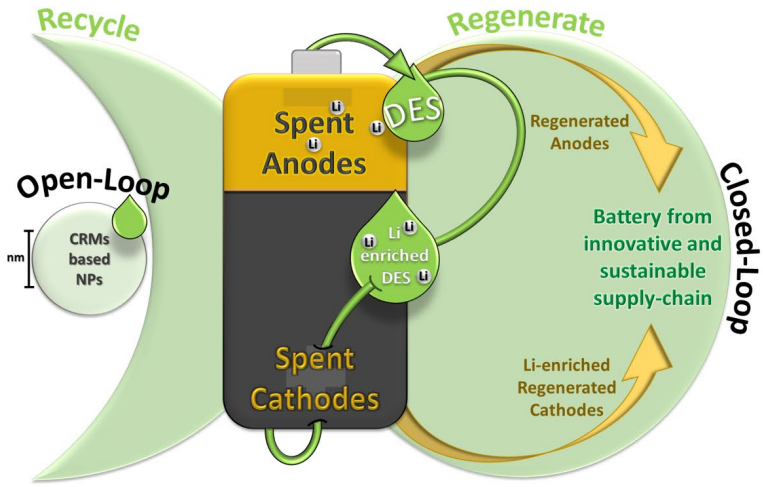

Fig. 4. Our recycling strategy for Spent Electrodes

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[2]Motta D. […], Bonomo M. Manuscript in preparation.

EES - D3 - P25

Commercial anion exchange membranes for alkaline water electrolysis: Linking performance, stability, and physicochemical properties

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Anion exchange membrane water electrolysis (AEMWE) combines the cost-effectiveness of alkaline systems with the efficiency of polymer electrolyte designs. However, the lack of standardized benchmarking hinders rational material selection and rational AEM design. This study presents a systematic evaluation of nine commercial AEMs (including Fumasep®, PiperION®, Selemion™, Sustainion®, and Xion™) under identical zero-gap conditions.
A comprehensive study of physicochemical properties—including ion exchange capacity (IEC), water uptake, hydration number, and swelling ratio—was conducted to establish structure-property relationships. The analysis reveals that performance is not dictated by IEC alone but by a delicate trade-off between conductivity and dimensional stability. PiperION® 40 µm and Sustainion® X37-50 emerged as top performers, reaching 2 $A \cdot cm^{-2}$ below 2.0 V at 60°C. Their success is attributed to self-supported structures that enable efficient ion transport through optimized hydration channels. In contrast, reinforced membranes exhibited increased ohmic resistance due to the tortuosity introduced by the support matrix, limiting their efficiency despite enhanced mechanical robustness.
Furthermore, ex-situ accelerated stress tests (1 M KOH, 80°C, 168 h) identified critical durability bottlenecks linked to polymer chemistry. The results demonstrated that ether-free backbones (e.g., poly(aryl piperidinium)) offer superior resistance to alkaline hydrolysis compared to aryl-ether based polymers, which suffered significant degradation. Additionally, imidazolium-functionalized membranes showed severe instability at elevated temperatures. These findings provide a vital, comparable dataset to guide the design of next-generation AEMs that simultaneously optimize conductivity, chemical stability, and operational lifetime.

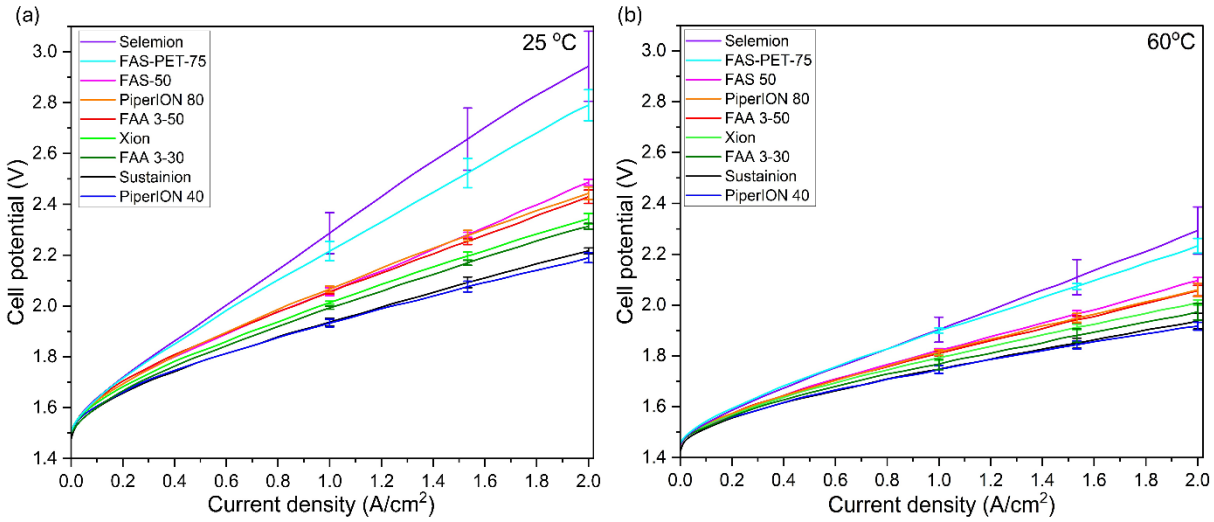

Fig. 1. Polarization curves of nine commercial AEMs measured in a zero-gap AEM water electrolyzer at 25 and 60 °C under identical operating conditions. Error bars represent the standard deviation of triplicate measurements.

This project was funded by the VLAIO ELECZIR project (no HBC.2023.0087)

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EES - D3 - P26
Is atmospheric half-life time of carbon tetrafluoride the same as it was 33 or 47 years ago?

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Carbon tetrafluoride (CF_4) is perhaps the most stable binary molecule. Nowadays CF4 is regarded as a potent climate gas with an estimated atmospheric lifetime of ≥50,000 years. This value is being reproduced in numerous background documents on climate change, in peer-reviewed papers and in non-scientific publications. The value comes from two independent estimates of Cicerone (1979)[1] and Ravishankara et al. (1993)[2]. Both estimates were based on a postulate that destruction of CF_4 in high-temperature combustion is the major way of its elimination. Naturally, the half-life time of 50,000 years was based on combustion data of late 70-s and early 90-s. Combustion of carbon fuel roughly doubled by 2026. This means the current value is obsolete and must be revised. Furthermore, the assumptions used[1,2] were rather weak and arbitrary. Analytical methods of today allow for inexpensive and accurate quantitation of CF_4. In combination with extensive knowledge on the scale and peculiarities of high-temperature combustion around the globe, it gives an opportunity to obtain an experimental value for atmospheric half-life time of carbon tetrafluoride in high-temperature combustion processes for science-based assessment of its contribution to climate change. In the meantime, the interim value based on the original methods[1,2] in combination with the most recent data for combustion will be presented.

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EES - D3 - P27

Ultra-small Ru and Ni clusters for enhanced CO_2 methanation at ultra-low metal loadings

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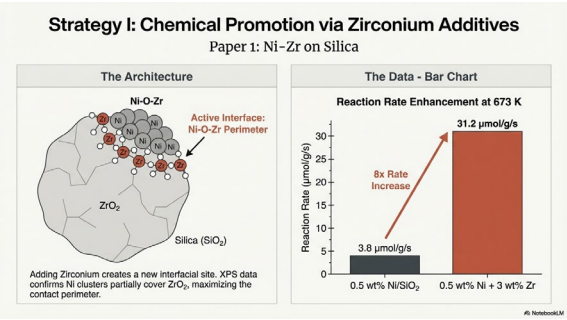
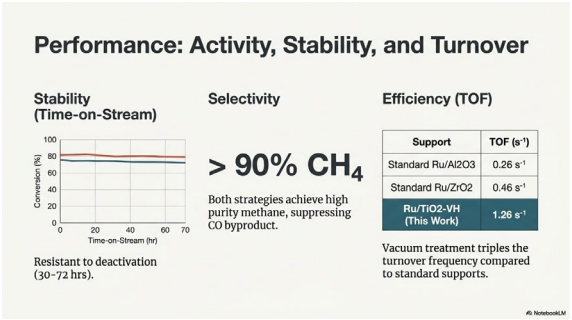
The catalytic hydrogenation of carbon dioxide to methane offers a promising route for renewable fuel production and carbon recycling. However, achieving high CO_2 methanation activity and CH_4 selectivity at low metal loadings remains challenging due to limited active site density and insufficient hydrogen activation. This study integrates two catalyst systems—Ru/TiO_2 and $Ni–Zr/SiO_2$—to demonstrate that the formation of ultra-small metal clusters is an effective strategy to enhance CO_2 methanation performance.For Ru/TiO_2 catalysts, a vacuum–hydrogen thermal pretreatment was applied to generate highly dispersed sub-nanometer Ru clusters at very low Ru loadings (0.5–1.0 wt%). This treatment strengthened metal–support interactions, increased surface oxygen vacancies, and promoted the formation of positively charged Ru species. As a result, CO_2 adsorption and hydrogen activation were significantly improved, leading to higher CO_2 conversion and near-complete CH_4 selectivity compared with conventionally prepared catalysts.

The findings demonstrate that atomic-scale Ru clusters can achieve excellent methanation efficiency without requiring high noble-metal content. In the Ni-based system, the introduction of Zr promoters onto low-loading Ni/SiO_2 catalysts (0.5 wt% Ni) created $Ni–ZrO_2$ interfacial sites that markedly enhanced catalytic performance. The Zr additive facilitated CO_2 binding and promoted hydrogen spillover to adjacent Ni clusters, shifting the reaction pathway from CO formation toward direct CH_4 production. These Ni–Zr catalysts exhibited improved CH_4 selectivity and lower activation barriers despite the minimal Ni content.

Overall, the results reveal that precisely engineered small Ru and Ni clusters with optimized metal–support interfaces maximize hydrogen coverage and CO_2 activation, enabling highly efficient CO_2 methanation at ultra-low metal loadings. This cluster-based design provides a sustainable approach for advanced carbon-neutral fuel synthesis.





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EES - D3 - P28

Optimization of operating parameters in single-stage membrane rotating biological contactor for wastewater treatment

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Membrane fouling remains a significant challenge that hinders the widespread adoption of membrane separation processes. This study focuses on optimizing the operating parameters of a novel membrane rotating biological contactor (MRBC), an integrated rotating biological contactor (RBC) and membrane filtration system within a bioreactor. The operating parameters (disk rotational speed, hydraulic retention time (HRT), and sludge retention time (SRT)) are optimized using the response surface methodology (RSM). RSM aimed to determine how operating parameters interact to affect filtration performance in the MRBC bioreactor. The results demonstrate that the MRBC achieved removal efficiencies of 84.4% for chemical oxygen demand, 97.1% for ammonium-N, and 43.9% for total nitrogen. RSM resulted in the highest membrane permeability of 456.7 L/m²·h·bar at a disk rotational speed of 35 rpm, 15 h HRT, and 15 days SRT. The proposed model closely matched the experimental data, with a coefficient of determination (R^2) of 0.988. Overall, this study presents a simple, feasible, and proof-of-concept strategy for constructing a compact MRBC design with the potential of minimizing membrane fouling. MRBC is a promising alternative to traditional wastewater treatment methods, offering a compact and efficient process that supports sustainable environmental practices and cleaner production development.

EES - D3 - P29

Matrix-specific partitioning of legacy and emerging PFAS in great tit (*Parus major*) plasma, feathers, and faeces near a fluorochemical hotspot

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Per- and polyfluoroalkyl substances (PFAS) are globally distributed, highly persistent contaminants,[1] yet the matrix-specific fate of emerging and novel PFAS in terrestrial food webs remains poorly understood. This study characterized PFAS occurrence, profiles, and partitioning in great tit (*Parus major*) plasma, feathers, and faeces along a contamination gradient surrounding the 3M fluorochemical plant in Flanders, Belgium. These were integrated with data on highly contaminated soils on the same area (ΣPFAS in soil previously reported up to 118 μg/g)[1] to infer bioavailability, accumulation, and elimination pathways. Targeted and suspect/non-target high-resolution mass spectrometry (SS/NTS-HRMS) revealed 137 individual PFAS from multiple classes. Matrix-dependent differences were evaluated with Kruskal–Wallis tests, with most PFAS showing highly significant partitioning and distinct concentration distributions across soil, plasma, feathers, and faeces.

Plasma was dominated by long-chain PFSAs, 80–100% detection frequencies, and relatively low within-matrix dispersion, consistent with strong protein binding and efficient systemic uptake. Whereas, feathers were enriched in PFESAs and unsaturated sulfonates. Faeces had consistently high detection (>70%) of many long-chain acids and sulfonates. Most of the PFAS showed significant matrix differences, and class-level plasma–soil correlations ranging from $\rho \approx 0.89$ to 0.98 for several legacy and emerging classes, including SF_5-PFSAs, PFESAs, and PFECAs. In contrast, weak class-level plasma–feather correlations indicated decoupling of internal dose and feather burdens. Principal component analyses separated soil, plasma, feathers, and faeces, suggesting combined plasma, feather, and faeces measurements as powerful bioindicators for PFAS biomonitoring at terrestrial hotspots.

Acknowledgements: We are grateful for the funding provided by the University of Antwerp and the Exposome Center of Excellence.

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EES - D3 - P30

Electrochemical dechlorination of PVC for sustainable materials recovery and the synthesis of chlorinated compounds

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Poly(vinyl chloride) (PVC) is one of the most widely used plastics and a major contributor to persistent waste streams. Its high chlorine content complicates conventional recycling and frequently leads to downcycling or incineration, with associated environmental impacts. In 2023, Anne J. McNeil and co-workers reported a plasticizer-mediated electro(de)chlorination strategy that enables PVC dechlorination directly from mixed plastic waste.[1] In this paired approach, chlorine equivalents released during dechlorination are leveraged in situ for selective arene chlorination, offering a compelling route to valorize plastic waste through synthetically useful chlorination chemistry. Building on this concept, we developed an electrochemical platform for PVC dechlorination that enables recovery and reuse of released chlorine for benzyl chloride synthesis (Figure 1). Mechanistic evidence[2,3] supports a mediated pathway in which an electrochemical mediator (MedE) is cathodically reduced to MedE•– and subsequently transfers charge to PVC, promoting selective C–Cl cleavage to form PVC• and Cl–. Chloride transport to the anode proved critical, as anodic oxidation generates reactive Cl• species that drive benzylic chlorination of toluene. By comparing divided and undivided cells and implementing biphasic reaction systems, we improved chloride management and benzylic chlorination selectivity while minimizing byproducts. Overall, this work demonstrates a circular "chlorine-loop" electrosynthetic strategy that couples PVC waste remediation with value-added chlorination chemistry, advancing sustainable plastics upcycling.

Fig. 1. Electrochemical dechlorination of PVC coupled to benzyl chloride synthesis.

We acknowledge financial support from Universidad de Alcalá (PIUAH25/CC-074),

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EES - D3 - P31

Rational design of amide-extended tetrahedral linkers for the construction of porous MOFs targeting CO_2 capture

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Metal-organic frameworks (MOFs) constructed from carboxylate-based linkers continue to demonstrate exceptional potential for applications in gas storage, separation, and catalysis.[1] In this work, we present the design and synthesis of highly branched amide-extended tetrahedral carboxylate linkers, developed by modifying previously established silicon-containing ligands that have been successfully employed within our research group.[2] Incorporating amide functionalities introduces additional sites for hydrogen bonding and guest interactions while enhancing linker rigidity and functionality.[3] These structural features facilitate the formation of robust, three-dimensional MOFs with well-defined porosity and high surface areas.

Several 3D MOFs were synthesized under solvothermal conditions and characterized by single-crystal X-ray diffraction, powder XRD, and spectroscopic techniques. The resulting frameworks display high crystallinity, permanent porosity, and excellent thermal stability. CO_2 uptake studies were performed at 273 and 298 K, revealing significant adsorption capacities consistent with the high surface areas and accessible functional sites of the frameworks.

This work highlights the potential of amide-functionalized derivatives of silicon-based linkers as a versatile platform for the rational design of functional MOFs for CO_2 uptake.

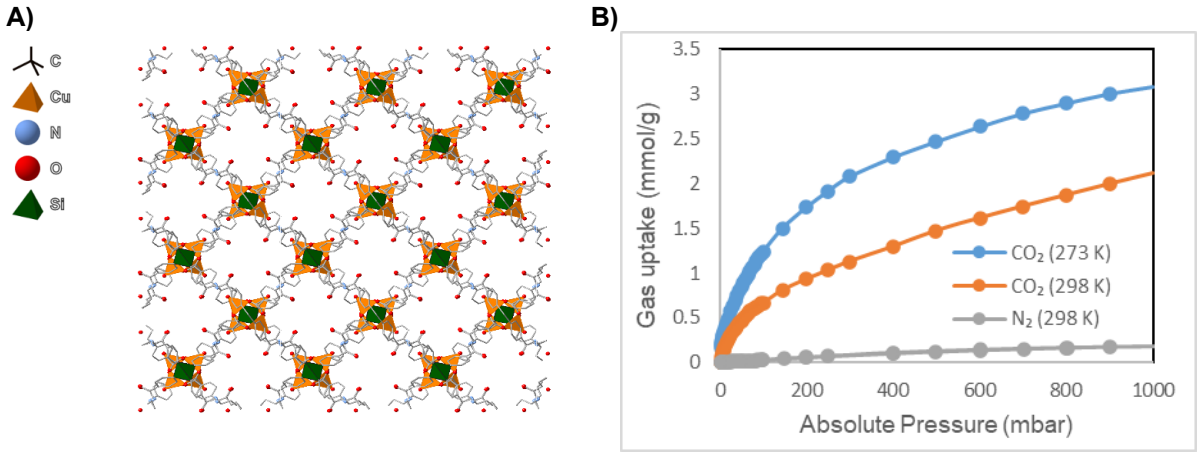

Fig. 1 Single-crystal X-ray diffraction (SXRD) of 3D MOFs A) Cu-MOF using a tetrahedral Si-centred linker B) CO_2 and N_2 uptake studies of the MOFs.

Acknowledgement: The authors gratefully acknowledge the **Commonwealth Scholarship Commission** for funding this research. We also thank **Schlumberger (SLB)** for their support and provision of resources that facilitated this study.

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EES - D3 - P32
Functionalized graphene oxide membranes for high flux nanofiltration

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Graphene oxide (GO) membranes have attracted significant interest for nanofiltration applications due to their tunable interlayer spacing and chemical versatility[1,2,3]. However, pristine GO membranes often suffer from extremely low water permeability (~1 $L.m^{-2}.h^{-1}.bar^{-1}$), which critically limits their practical utility[4]. In this work, we demonstrate a substantial performance breakthrough by functionalizing GO with a covalent organic framework (COF) assembled from the cationic monomer ethidium bromide and 1,3,5-triformylphloroglucinol. The intercalation of the cationic COF within GO nanosheets effectively tunes and stabilizes the interlayer channels, creating well-defined transport pathways for water molecules while simultaneously enhancing electrostatic interactions with target solutes (Figure 1). As a result, the functionalized membranes exhibit an ultrahigh water flux of 73.5 $L.m^{-2}.h^{-1}.bar^{-1}$, over 70-fold higher than pristine GO, while maintaining excellent rejection toward low molecular weight organic compounds. This remarkable synergy arises from the combined effects of (i) improved interlayer spacing uniformity, (ii) increased hydrophilicity and charge-assisted transport, and (iii) strong size- and charge-based selectivity[5,6]. The structural incorporation of the COF within the GO lamellar architecture was unambiguously confirmed by X-ray diffraction, Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy, and electron microscopy, among other techniques, affirming the successful construction of the hybrid framework. Overall, this strategy illustrates a powerful route to overcoming the permeability–selectivity trade-off in GO-based membranes, enabling their deployment for high-efficiency nanofiltration of challenging organic micropollutants. Our findings highlight the potential of rationally designed GO–COF composites as scalable, high-performance membrane materials for next-generation water treatment technologies.

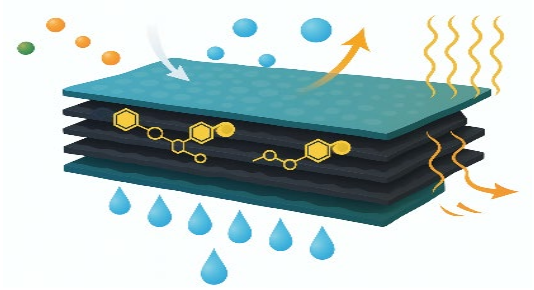

Fig.5. Schematic illustration of EtBr COF-functionalized GO membrane showing enhanced ion sieving and water permeance.

Acknowledgement: The authors would like to acknowledge the support provided by King Fahd University of Petroleum and Minerals, Interdisciplinary Research Center for Membranes & Water Security (project # INMW2512).

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EES - D3 - P33
Oxidative denitrogenation using sustainable carbon nanotubes: Reactive oxygen species

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Oxidative denitrogenation (ODN) is a process that allows removing undesired N species from fuels[1]. H_2O_2 is the main oxidant source[1], which should be decomposed into reactive oxygen species by proper catalysts to achieve suitable reaction rates. Another current issue is the accumulation of plastic solid waste (PSW), which can be upcycled into carbon nanotubes (CNTs), thus substituting fossil-derived precursors in the obtention of advanced materials[2]. In this work, CNTs were synthesized from polymers, following the procedures detailed here[2] for POL-OX@NiFe synthesis. The CNT was used as catalyst for ODN of quinoline (QN). QN (in aqueous and oily phases) and H_2O_2 were monitored. tert-butanol and p-benzoquinone were used as indirect probes for $HO^{\bullet}$ and $O_2^{\bullet-}$ (Figure 1). The addition of tert-butanol (50 mM) caused a pronounced decrease in QN oxidation, reducing global removal after 2 h from ca. 90 to ~40%, confirming that $HO^{\bullet}$ are relevant oxidizing species. The addition of p-benzoquinone (10 mM) caused a milder inhibition (QN removal at 2 h of ~66%), suggesting that $O_2^{\bullet-}$ participate as secondary oxidants.

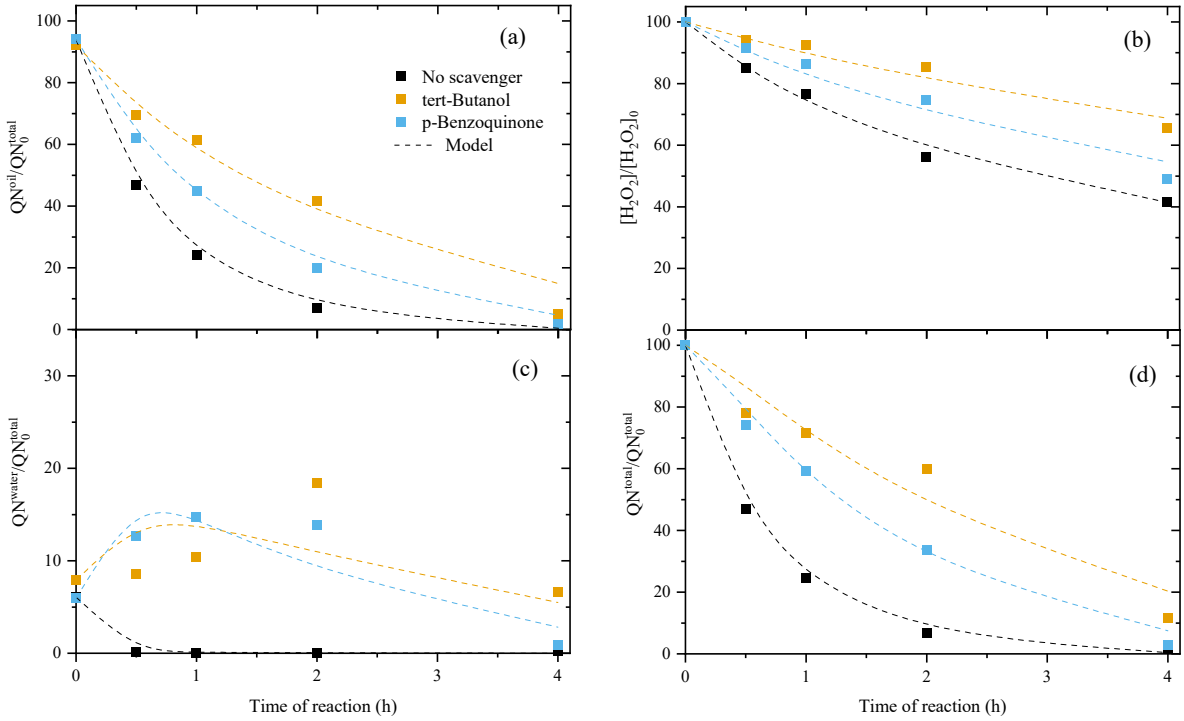

Fig.1. (a) QN removal from fuel, (b) H_2O_2, (c) QN in aqueous phase and (d) overall QN abatement. Conditions: $[QN]_0$ = 500 mg L^{-1} in 2,2,4-trimethylpentane, $[H_2O_2]_0$ = 12 g L^{-1}, O/W volume ratio = 80:20, T = 70 °C, [POL-OX@NiFe] = 2.5 g L^{-1}, pH_0 = 3.0. Dashed lines represent the kinetic model described elsewhere[3]

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO (DOI: 10.54499/UIDB/00690/2020 and 10.54499/UIDP/00690/2020) and SusTEC (DOI: 10.54499/LA/P/0007/2020); and by *Sociedade Ponto Verde* with the project "*Estudo técnico-económico para a valorização de resíduos de embalagens plásticas na produção de nanotubos de carbono*".

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EES - D3 - P34
Removal of bisphenol-A by catalytic wet peroxide oxidation using sustainable carbon nanotubes

Thoriso Kotsoane[1], Adriano Silva[1], Helder T. Gomes[1], Fernanda F. Roman[1]
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Typical wastewater plants fail to remove compounds found in the ng/L - µg/L range[1], resulting in a pressing need to develop low-cost solutions for the removal of human-use substances (HUS)[1]. In this context, catalytic wet peroxide oxidation (CWPO) is a hydroxyl radical-based technology that can eliminate a wide range of HUS at mild operating conditions given that active catalysts are used[2]. Another current issue is the generation and accumulation of plastic solid waste (PSW), which can be upcycled into carbon nanotubes (CNTs), thus substituting fossil-derived precursors in the obtention of advanced materials[3]. In this work, a CNT was synthesized from PSW provided by the local waste management company. More details about synthesis conditions can be found here[3]. The CNT was used as catalyst on the CWPO of bisphenol-A (BPA) as a microplastic representative. The waste-derived CNT demonstrated high catalytic activity, which when compared to the non-catalytic run (NC) resulted in a 2.5× and 63× increase in BPA removal and H_2O_2 consumption, respectively, at 2 h of reaction. High TOC removals and efficiency of H_2O_2 consumption ($\eta_{H_2O_2}$) were achieved in the presence of the CNT, as shown in Figure 1.

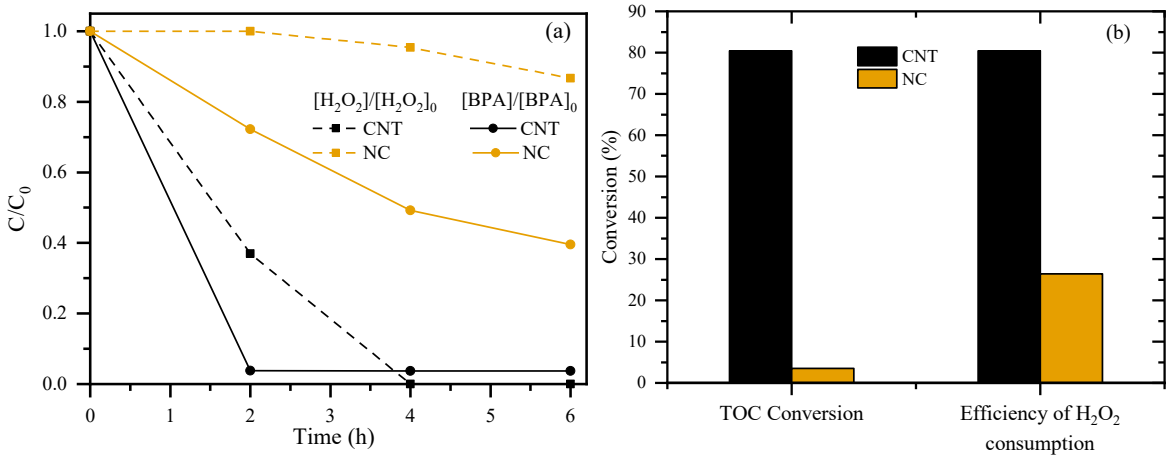

Fig.1. (a) CWPO of BPA and (b) TOC conversion and $\eta_{H_2O_2}$. Conditions: $[BPA]_0$ = 100 ppm, $[H_2O_2]_0$ = 536 ppm, pH_0 = 3.5, T = 80 °C, C_{cat} = 2.5 g L^{-1}. NC in the absence of hydrogen peroxide.

This work was supported by national funds through FCT/MCTES (PIDDAC): CIMO (DOI: 10.54499/UIDB/00690/2020 and 10.54499/UIDP/00690/2020) and SusTEC (DOI: 10.54499/LA/P/0007/2020); and by *Sociedade Ponto Verde* with the project "*Estudo técnico-económico para a valorização de resíduos de embalagens plásticas na produção de nanotubos de carbono*".

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EES - D3 - P35
Electrochemical approach towards the total synthesis of (-)-colchicine

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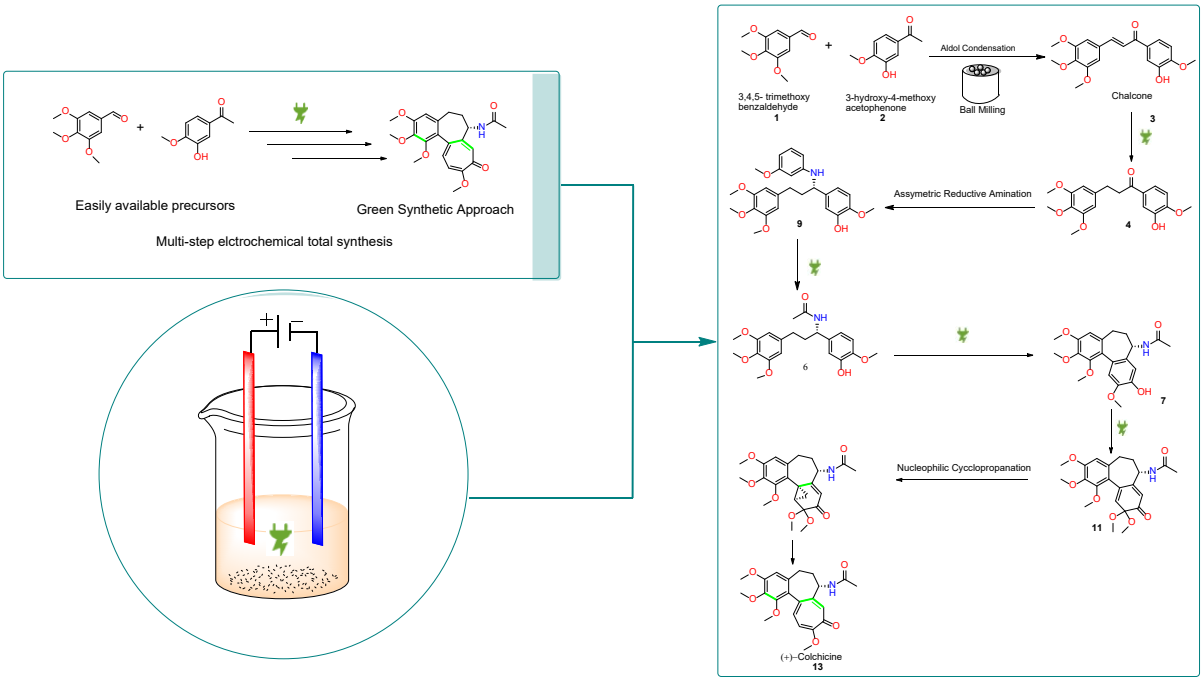
Loughborough University, UK

Colchicine is a pharmaceutically important alkaloid whose total synthesis remains challenging due to its structural intricacy and stereochemical complexity. In this study, we report a sustainable electrochemical strategy for the synthesis of (-)-colchicine, aiming to replace hazardous reagents while improving overall process efficiency. In the asymmetric synthetic pathway, four of the eight steps were performed electrochemically, including electrochemical reduction, intramolecular cyclisation, deprotection, and dearomatisation reactions. In addition, the synthetic route incorporates a solvent-free mechanochemical transformation and an asymmetric reductive amination step to introduce enantiopurity. Collectively, these methodologies provide a more sustainable and environmentally benign approach to the total synthesis of colchicine. The electrochemical transformations proceeded in moderate to high yields, demonstrating the potential of electrochemical techniques to enhance yield, selectivity, and operational safety. This work highlights the promise of electrochemical synthesis as a green and efficient platform for constructing complex natural products.



EES - D3 - P36

Nano-calcium driven degradation of dichlorodiphenyltrichloroethane in soil: Efficiency assessment and underlying mechanisms

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Dichlorodiphenyltrichloroethane (DDT) introduced in the 1940s as an effective insecticide, has since become recognized as a globally persistent organic pollutant. Its chemical stability, strong adsorption to soils, and ability to bioaccumulate allow DDT and its metabolites particularly DDE and DDD to persist in ecosystems for decades. Despite widespread regulatory restrictions and bans, DDT residues remain detectable worldwide, highlighting the need for effective remediation strategies.

This study evaluated the degradation of DDT in low-moisture Akadama sandy soil (5.1% moisture),(a granular volcanic soil widely used in Japan), artificially contaminated with 100 mg of DDT per 100 g of soil. Using a ceramic grinding mortar equipped with a rotary stirring system (40 rpm), 5 g subsamples of the spiked soil were treated with nano-calcium (nCa) at dosages of 0.5 g and 5 g for 1 h and 24 h under both air and nitrogen atmospheres. Post-treatment, DDT leaching tests were conducted using 50 mL of toluene for extraction, followed by quantification via GC-MS.

Results demonstrated that the highest degradation efficiency of 92% was achieved under aerobic conditions with 5 g nCa, compared to 75% under nitrogen. The lower dosage of 0.5 g nCa resulted in similar efficiencies 64% across both atmospheric conditions. Depending on each country: WHO guideline threshold of 1 g/m². nCa dosage emerged as the dominant factor influencing degradation, whereas stirring time showed minimal effect under aerobic conditions and only slight improvement under nitrogen. Overall, nCa exhibited strong potential as a soil remediation agent for DDT-contaminated environments. Further studies are recommended to optimize treatment parameters and elucidate the dechlorination pathways driving nCa-mediated DDT breakdown.

Acknowledgements: This research was supported by the SICORP program of the Japan Science and Technology Agency (JST) under the Africa–Japan Collaborative Research (A-J CORE) initiative. It was conducted as part of the project “Sustainability Challenge in Africa: Purification of Contaminated Soil Using Nano-Calcium and Its Recycling into Eco-Fertilizer and High-Strength Concrete (SCA-CEFC).

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EES - D3 - P37

Non-stoichiometric CuAgSe doped with Zn or Fe: Mechanochemical synthesis and thermoelectric properties

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Thermoelectric materials can convert heat to electricity and vice versa, offering a potential way to utilize waste heat. Among functional thermoelectric materials are also metal chalcogenides, including ternary CuAgSe. The application of environmentally friendly synthetic methods is an increasingly important factor in chemistry nowadays. Ball milling offers a simple, one-pot, solvent-free, time-saving method at room temperature and ambient pressure.

This study was performed in order to investigate the influence of doping by various amounts of zinc or iron on the thermoelectric properties of non-stoichiometric $Cu_{2-x}Ag_xSe$. Previously published works differ in (non-)stoichiometry of CuAgSe, in selected dopant, and in synthesis method, but similarly show significant changes in thermoelectric properties of doped CuAgSe.[1,2]

Mechanochemical syntheses of $Cu_{0.6}Ag_{1.4}Se$ doped with 3, 6, 10% of Zn or Fe over Cu were carried out in a planetary ball mill Pulverisette 6 (Fritsch, Germany) from elemental powders. Syntheses were completed after only 7 min of milling, which was confirmed by XRD analysis. For the consolidation of the prepared powders into pellets, the SPS method was used. The phase composition, morphology, specific surface area, mean particle size, and thermoelectric properties of the samples have been studied.

Acknowledgement: This work was supported by the Slovak Grant Agency VEGA (project 02/0036/23) and the Slovak Research and Development Agency (contract no. APVV-24-0353).

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EES - D3 - P38

Magnetic heating-assisted methanol synthesis from CO_2 and H_2 for Power-to-X applications

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Methanol is the simplest aliphatic alcohol and is widely used as a solvent, fuel, and energy storage medium. In addition to its traditional applications, methanol is receiving increasing attention in Power-to-X (PtX) technologies, which convert excess renewable energy into chemical energy. In this context, methanol can be produced from captured CO_2 and H_2 obtained via water electrolysis. Producing carbon-neutral fuels is not only beneficial for the environment but also enables more efficient energy storage and allows seamless integration into the existing fuel infrastructure. Thus, methanol is a promising energy carrier for the storage and transportation of renewable energy.[1-2]

In this study, methanol synthesis was carried out using magnetic heating, a process that relies on an alternating magnetic field (AMF) to induce localized and rapid heating in ferromagnetic nanoparticles. To achieve this, a magnetic nanocomposite consisting of CoFe nanoparticles and a silica-alumina shell was prepared. This magnetic support was used to prepare the methanol catalyst by coprecipitating copper and zinc onto the silica-alumina shell, yielding the final catalysts for methanol synthesis.

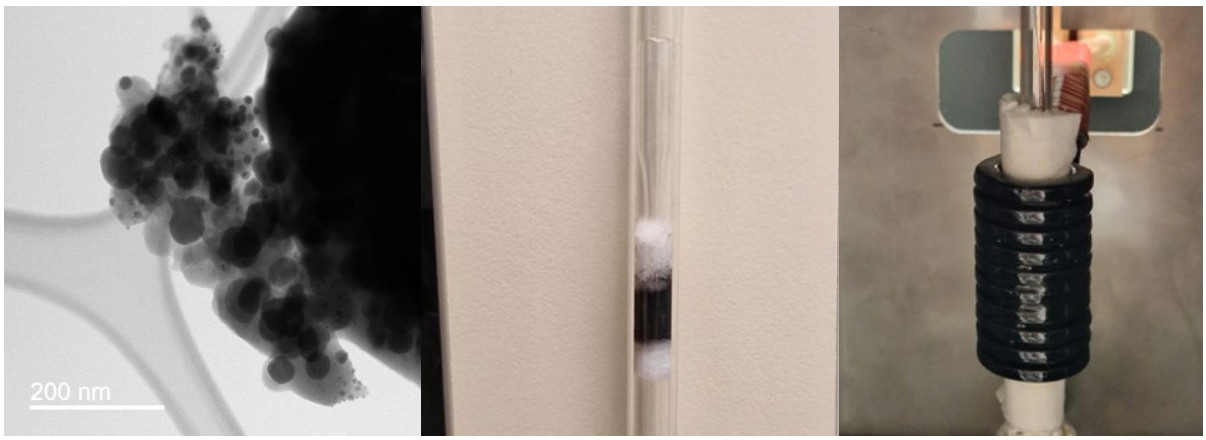

Fig. 6. Left: STEM image of CoFe nanoparticles within a silica-alumina shell. Middle: quartz reactor containing the catalyst. Right: induction coil placed around the reactor for magnetic heating.

Catalytic experiments were conducted in a fixed-bed induction reactor using 200 mg of catalyst and a constant gas flow of 50 mL/min (H_2: CO_2 = 3:1) at 30 bar and temperatures between 200 and 300°C. At 250°C, 0.5 mol% methanol was detected in the gas phase with very high selectivity. This can be attributed to the silica-alumina shell, which acts as a barrier and suppresses undesired side reactions, such as methanation and Fischer-Tropsch synthesis, of the magnetically heated CoFe cores. These results demonstrate the feasibility of methanol synthesis via magnetic heating and highlight its potential for PtX applications.

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EES - D3 - P39

Water-induced structural deactivation of zeolite-supported magnesium chloride and its effect on ammonia sorption stability

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Ammonia is emerging as a carbon-neutral energy carrier, but its conventional production remains energy intensive[1]. Solid sorbents, especially metal halides, offer a promising alternative to conventional ammonia separation by condensation. Magnesium chloride is especially attractive for ammonia separation and storage applications due to its strong and reversible coordination with ammonia[2]. However, its practical application is still limited by structural instability and high sensitivity to moisture[3], motivating a deeper understanding of its degradation behaviour.

This study provides a mechanistic and quantitative assessment of moisture- and cycling-induced degradation of $MgCl_2$-impregnated ultra-stable Y (USY) zeolite[4]. Using FTIR and XPS analysis, it was found that water exposure progressively deactivates $MgCl_2$ active sites through the formation of oxygen-containing magnesium species, including MgO and MgOHCl. Pre-ammoniation of the material with ammonia and density functional theory calculations provide evidence that pre-adsorbed ammonia does not inhibit water absorption and demonstrate that ligand exchange reactions are thermodynamically favoured over molecular water intercalation, clarifying the degradation pathway. Temperature-programmed desorption measurements reveal that co-exposure to ammonia and water modifies the magnesium coordination environment, which weakens ammonia binding. Furthermore, ammonia cycling under dry conditions was also investigated. The results show that ammonia cycling causes irreversible structural changes through the formation of defect-rich crystalline regions that reduce ammonia capacity. Despite these degradation mechanisms, sorption experiments demonstrate that $MgCl_2$/USY maintains a measurable ammonia uptake at high-temperature (300 °C, 8 bar), indicating potential for use in integrated ammonia sorption-enhanced ammonia synthesis. These findings help establish operational limits for the practical application of supported magnesium chloride sorbents.

The work was funded by the European Union – Horizon Europe, Grant Agreement [101058643], HySTrAm: Hydrogen Storage and Transport using Ammonia, and by the Slovenian Research and Innovation Agency through core funding P2-0152, infrastructure funding I0-0039, and the research projects N2-0291 and TN-03. The research was (co-)funded under the HyBReED project, supported by the European Union – NextGenerationEU. Computational resources at the HPC system Vega at the Institute of Information Science, Maribor, Slovenia were provided by the HPC RIVR consortium and EuroHPC JU.

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EES - D3 - P40

Redox electrolyte-assisted hybrid energy storage with optimized cathode/anode ratio of cobalt hexacyanoferrate and activated carbon

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Hybrid energy storage devices combine a battery-type (faradaic) electrode with a capacitive-type electrode to simultaneously achieve high energy and power densities. However, mismatches in reaction kinetics and charge storage capacity can deteriorate both energy and power densities. Here, an open-framework cobalt hexacyanoferrate (CoHCF) cathode is introduced to enable rapid Na^+ insertion/extraction kinetics compatible with the capacitive-type electrode, thereby mitigating the kinetic mismatch in a hybrid energy storage system.

Activated carbon (AC) was employed as the anode, and heptyl viologen dibromide ($HVBr_2$) was used as the redox-active electrolyte. During charging, Na^+ ions deintercalate from the CoHCF cathode, while the anode accommodates Na^+ adsorption on activated carbon accompanied by the reduction of HV^{2+} species (Fig. 1). To resolve capacity mismatch, hybrid cells with different cathode-to-anode mass ratios were systematically designed and evaluated. As a result, the optimized CoHCF//AC hybrid cell with a cathode-to-anode mass ratio of 1:2 delivered a maximum power density of 516 W kg^{-1} and an energy density of 44 Wh kg^{-1}.

The $HVBr_2$ electrolyte contributes to anode-side charge storage through reversible redox reactions. Upon reduction, the resulting HV species ($HV^{\bullet+}$) adsorb on the anode surface to form a surface film that suppresses self-discharge, leading to a capacity retention of 78% after 72 h. Through rational material selection and device design, this work demonstrates a hybrid energy storage system that simultaneously overcomes kinetic and capacity mismatches between electrodes while delivering high energy and high power densities. The proposed hybrid device shows strong potential for applications requiring rapid charge–discharge operation combined with high energy storage capacity.

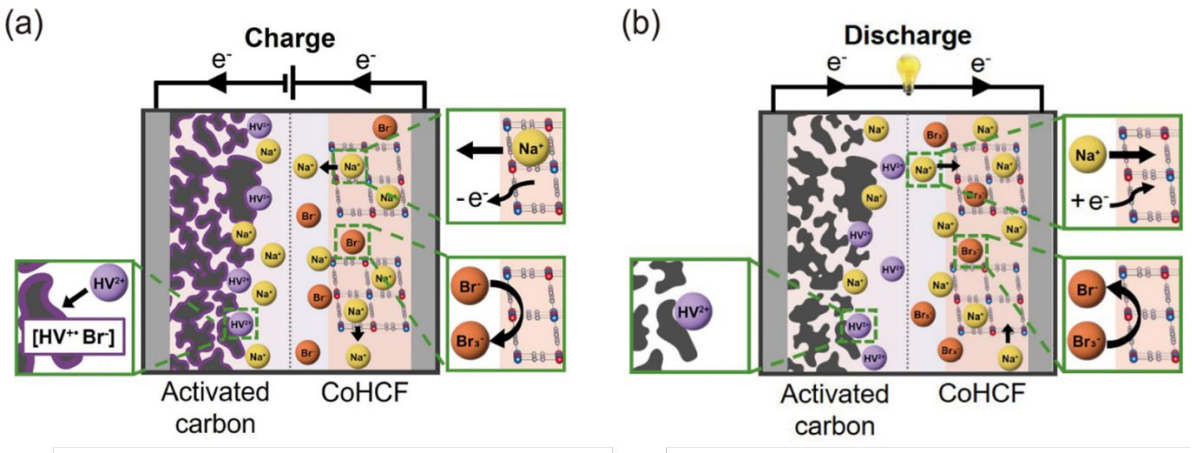

Fig. 1. Schematic illustration of the energy storage mechanisms in a hybrid energy storage device under (a) charged and (b) discharged states

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EES - D3 - P41
Silk fibroin solid electrolyte membranes for sustainable sodium-ion batteries

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The growing demand for sustainable and cost-effective energy storage technologies has intensified interest in sodium-ion batteries as an alternative to lithium-based systems, owing to the natural abundance and wide geographical distribution of sodium. However, the development of safe and efficient solid-state electrolytes remains a critical challenge for the practical implementation of sodium-ion batteries.
In this work, silk fibroin is explored as a bio-based polymer matrix for the development of solid electrolyte membranes tailored for sodium-ion battery applications. Silk fibroin is a renewable and biodegradable biopolymer that combines excellent film-forming ability, mechanical robustness, and structural tunability, making it particularly attractive for solid-state electrochemical devices. By incorporating sodium salts and selected plasticizing agents, flexible fibroin-based membranes with enhanced ionic transport properties are obtained.
The resulting solid electrolyte membranes exhibit ionic conductivities in the 2 $mS \cdot cm^{-1}$ range at ambient temperature and high humidity, together with good thermal stability and structural integrity. The relationship between fibroin molecular structure and ion transport is discussed, highlighting the role of polymer chain organization and amorphous domains in facilitating sodium-ion conduction. These results demonstrate that silk fibroin-based electrolytes are a promising sustainable platform for the development of safer and environmentally friendly solid-state sodium-ion batteries.

Fig. 1. Silk Fibroin as polymer electrolyte membrane.

Acknowledgements: This work was financed by the BioEESC project (COMPETE2030-FEDER-00779500) and within the scope of the project CICECO-Aveiro Institute of Materials, UID/50011 & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC), financed by national funds through the FCT/MCTES (PIDDAC). Acknowledgments are also due to FCT/MCTES for the P. Barbosa (2023.06523.CEECIND) contract.

EES - D3 - P42

High-temperature structural and microstructural evolution of Ni- and Mn-doped $LaCoO_3$ perovskites

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[1]Ruđer Bošković Institute, Croatia; [2]Central European Institute of Technology, Brno University of Technology, Czech Republic

$LaCoO_3$ perovskites are beneficial for photovoltaics, catalysis, and energy storage due to their chemical stability and resilience.[1,2] Cooperative rotations of oxygen octahedra give its crystal structure trigonal symmetry, derived from the ideal cubic perovskite ABX_3 (A = La^{3+}, B = Co^{3+}, X = O^{2-}). Transition metal doping at A- and/or B-sites enhances structural and electrical characteristics, revealing new functions.

We investigates the structural evolution of $LaCoO_3$, $LaCo_{1-x}Ni_xO_3$ (x = 1.3 at.%, 2.9 at.%), and $LaCo_{1-x}Mn_xO_3$ (x = 1.7 at.%, 2.8 at.%) at temperatures up to 1000 °C, focusing on cation distribution at various temperature intervals using laboratory X-ray diffraction during controlled heating and gradual cooling. In addition to assessing diffraction line broadening, we explain temperature-induced variations in the oxygen positional parameter, La–O and Co/Ni(Mn)–O distances, and Co/Ni(Mn)–O–Co/Ni(Mn) angles calculated from structural refinements. Field-emission scanning electron microscopy micrographs of samples before/after slow cooling show reveal the effect of thermal treatment. Diffraction patterns showed that all samples were nanocrystalline and retained the *R*-3*c* space group's hexagonal axes within the temperature range. Ni- and Mn-doped $LaCoO_3$ exhibited increased unit cell parameters and diffraction line broadening under ambient conditions; however, cation distribution did not change significantly with temperature. Heating $LaCoO_3$ and Ni- and Mn-doped $LaCoO_3$ perovskites to 1000°C, followed by cooling to ambient temperature, enhances the resolution of hexagonal structure-related doublet peaks in powder XRD patterns. At elevated temperatures, $LaCoO_3$ exhibits dynamic oxygen octahedral rotations resulting in a higher-symmetry pseudo-hexagonal arrangement that improves lattice coherence and crystallite ordering during cooling. Heating reduces microstrain, sharpening doublet reflection splitting and significantly alters oxygen positional features and metal-oxygen distances, which control this perovskite family's catalytic and electrical capabilities.

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EES - D3 - P43

Controlled autoxidation of heavy petroleum residues as a low-cost route to synthesize carbon nanotubes

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Carbon nanotubes (CNTs) demand is growing globally at a CAGR of 13.6% due to their wide range of industrial applications, including reinforcement fillers in composites, conductive additives in batteries and supercapacitors, electromagnetic interference shielding materials, sensors, membranes, and catalyst supports. Conventional CNTs are commonly synthesized from methane or acetylene via chemical vapor deposition, arc discharge, or laser ablation, at a production cost of approximately $10–50 per gram. On the other hand, heavy petroleum residues provide a low-cost ($1 per kg), carbon-rich, and more environmentally friendly alternative. This study explores heavy oil residues derived asphaltenes as low-cost alternative precursors for CNTs synthesis. The residues were subjected to controlled autoxidation via air blowing without mixing at relatively low temperatures (≤280 °C) for varying durations. Following oxidation, asphaltenes were isolated using n-heptane as the precipitating solvent and subsequently employed as precursors for carbon nanotube synthesis via a template-assisted pyrolytic growth method. Controlled free-radical oxidation enhances precursor properties, including increased viscosity, reduced volatility, changes in elements and functional groups, changes in molecular weights and improved cross-linking, and higher softening point and aromaticity. The synthesized CNTs were characterized using SEM, XRD, and Raman spectroscopy analyses. During SEM analysis, CNTs exhibited an aligned CNT growth and bundled multi-walled CNTs with diameters ranging from ~50 to 200 nm. XRD confirmed the formation of partially graphitized, turbostratic multi-walled CNTs. From the relative intensities of the Raman G and D bands, the degree of graphitization of the produced CNTs were estimated as IG/ID ≈ 0.9–1.2, indicating improved graphitic ordering and reduced defect density upon oxidation pretreatment. These findings demonstrate a promising route for converting low-value petroleum residues into CNTs, supporting economic diversification of refinery by-products, while emphasizing the need for further optimization of graphitization and purity to enable large-scale, high-performance applications.

Keywords: Carbon nanotubes; Heavy vacuum gas oil; Precursors; Autoxidation (air blowing); Sustainable materials.

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EES - D3 - P44

Optimizing solvent roles in catalytic lignin liquefaction: Efficient pathways to phenolic monomers and bio-oil

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Lignin, one of the three major components of lignocellulosic biomass, is generated as a byproduct of pulping and bioethanol industries, with an estimated annual production of about seven million tons. Despite its abundance, lignin remains largely underutilized, yet it represents a promising renewable feedstock for the production of biofuels, phenolic monomers, and other value-added chemicals. Among emerging conversion pathways, liquefaction has gained attention as an effective route for transforming technical lignins, such as Kraft lignin, into high-quality liquid products. In this study, the effects of key liquefaction parameters, including temperature, reaction time, and solvent type, on lignin depolymerization were systematically investigated under supercritical conditions. Product yield, composition, and quality were evaluated using GC-RGA, GC-SIM-DIS, GC–MS, thermogravimetric analysis, and elemental analyses. Catalytic upgrading was performed using a Ni-based catalyst in supercritical alcohols without the use of an external hydrogen source, enabling a more sustainable upgrading strategy. The use of supercritical alcohols facilitated simultaneous depolymerization, esterification, hydrogenation, decarbonylation, and decarboxylation reactions, resulting in a significant reduction in oxygen content and an increase in the higher heating value of the produced bio-oils. Particular emphasis was placed on maximizing the yield of phenolic monomers, which are important intermediates for fuels and chemical synthesis. Short-chain alcohols (C_1–C_3) served as both solvents and hydrogen donors, promoting in situ hydrogen generation and suppressing char formation. Under optimized reaction conditions, solvent consumption was substantially reduced while maintaining high product selectivity and stability. Catalyst performance and structural stability were examined using transmission electron microscopy, N_2 physisorption, and X-ray diffraction. The upgraded oils were further analyzed to determine phenolic monomer distribution, overall yield, and energy content. The results demonstrate that supercritical alcohols provide an efficient and sustainable medium for lignin depolymerization, offering mechanistic insight into solvent–lignin interactions and a viable pathway for lignin valorization toward renewable fuels and chemicals.

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EES - D3 - P45
Solvent-free upcycling of plastic waste to aromatics with multi-shelled hollow sphere

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Typically, a metal oxide-zeolites catalyst is usually produced either by physically mixing metal oxide nanoparticles as dopants with the zeolite substrate, or by an impregnation process, resulting in an architecture, where metal oxide nanoparticles are dispersed randomly on the zeolite.[1] As a result, the uneven distribution of metal oxides on zeolites catalyzed the conversions instantly rather than sequentially. Furthermore, the metal oxides and zeolites components typically catalyze the initial and subsequent reactions in the tandem catalysis process to yield aromatics and the products created in the first stage on the metal oxide site may diffuse out without undergoing further reactions on the zeolite phase. Therefore, a random architecture is not optimal for achieving the highest efficiency and desired sequence in the tandem reaction. In addition, aromatization requires adequate acid sites (both Brønsted and Lewis) and shape-selective microporous structures to facilitate the complex reaction cascade (cracking, oligomerization, cyclization, dehydrogenation). We propose a generally applicable and simple synthesis method for facet-controlled nanocrystals@metal oxides@zeolites multi-shelled hollow spheres with predetermined metal-zeolite spatial organization and short diffusion length as illustrated in Figure 1. The developed preparation method allows control over different structural parameters and chemical compositions. The step-by-step conversion from the precursor material to the final solid catalyst will be monitored and the essential mechanisms for the involved self-assembly and hollowing behaviors will be revealed. We believe that the proposed synthesis has numerous advantageous and has potential to outperforms the conventionally synthesized materials via precipitation and impregnation procedures in the selective production of aromatics by upcycling of plastic waste. We will demonstrate that each structural engineering element in nanocrystals@metal oxides@zeolites multi-shelled hollow spheres, including the hollow-sphere design, core-shell spatial organization and “cage” effect of the H-ZSM-5 shell, contributes to the improvement of catalytic performance.

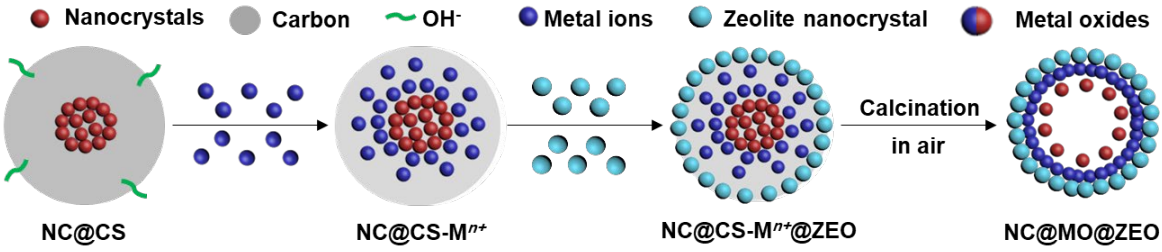

Fig. 1. Schematic illustration of the synthesis of nancrystals@metaloxides@zeolites hollow spheres

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EES - D3 - P46
Shrimp shell waste as a green resource for rare earth element recovery

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The growing demand for rare earth elements (REEs), driven by their essential role in clean energy technologies such as wind turbines and electric vehicles, raises critical supply, environmental, and geopolitical concerns[1]. NdFeB permanent magnets, containing REEs such as Nd, Pr, Dy, and Gd, generate significant waste both during manufacturing (15–30%) and at end-of-life (EoL)[2,3], highlighting the need for sustainable recovery strategies aligned with circular economy principles.
This study investigates shrimp shells (SS), an abundant and low-cost seafood-processing biowaste, as a natural biosorbent for the selective recovery of REEs from multi-element solutions simulating leachates of EoL NdFeB wind turbine magnets. Batch sorption experiments were conducted under varying pH, salinity, ion concentration, and sorbent dosage using synthetic solutions containing B, Ni, Co, Nd, Dy, Pr, and Gd at 100 µM.
Untreated shrimp shells outperformed thermally treated materials (400–600 °C), achieving >98–99% REEs removal while limiting the co-removal of competing metals such as Co (≈28%), Ni (≈27%), and B. Response surface methodology identified sorbent dosage and initial ion concentration as the most influential parameters, with optimal REEs selectivity at pH 3.0 and no significant effect of salinity. Under optimised conditions, 80–85% of REEs were selectively removed from simulated magnet leachates.
Kinetic studies showed rapid adsorption, reaching equilibrium within 6 h, with the Elovich model providing the best fit. Equilibrium data followed the SIPS isotherm, yielding maximum adsorption capacities of 75.5–89.7 mg/g. Desorption experiments demonstrated that dilute nitric acid (0.1 M) enabled >85% recovery of adsorbed REEs.
Overall, this work highlights raw shrimp shell waste as an efficient, selective, and sustainable biosorbent for REEs recovery from complex secondary resources.

Acknowledgement: This work received financial support from PT national funds (FCT/MCTES, Fundação para a Ciência e Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) through the REQUIMTE (UID/50006 – Laboratório Associado para a Química Verde – Tecnologias e Processos Limpos) and CICECO-Aveiro Institute of Materials (UIDB/50011/2020 & UIDP/50011/2020). This work is funded by COMPETE2030-FEDER-00847800. Nicole Ferreira thanks the Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior for their PhD grant ref. 2022.13017.BD. Thainara Viana thanks the Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior for their PhD grant ref. 2022.13015.BD.

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EES - D3 - P47

Synthesis and catalytic evaluation of $NiO–Al_2O_3$ catalyst for steam methane reforming

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Hydrogen serves as a crucial energy carrier in the shift to low-carbon and sustainable energy systems, with uses in clean power generation, chemical processing, and fuel cell technology. Steam methane reforming (SMR) remains the most important industrial method for hydrogen production; however, developing efficient, stable, and cost-effective catalysts is vital to enhance process performance and hydrogen output. In this study, a $NiO–Al_2O_3$ catalyst was created using a controlled chemical process and thoroughly characterized to evaluate its suitability for SMR.

The synthesized catalyst was characterized using X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, scanning electron microscopy (SEM), and temperature-programmed techniques to elucidate phase composition, surface properties, and metal–support interactions. Catalytic performance was evaluated in a fixed-bed reactor under steam methane reforming conditions. The $NiO–Al_2O_3$ catalyst demonstrated excellent activity, achieving 99 % methane conversion with a high hydrogen yield under the investigated operating conditions.

The enhanced performance is attributed to the high dispersion of NiO species on the Al_2O_3 support, strong metal–support interactions, and favorable surface characteristics that promote efficient methane activation. A clear correlation between synthesis, structural features, and catalytic performance is established. These results highlight the potential of $NiO–Al_2O_3$ as an effective catalyst for hydrogen production via steam methane reforming.

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EES - D3 - P48

Synthesis and evaluation of porous organic polymers for CO_2 capture

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The burning of fossil fuels has been a continuous contributor to atmospheric levels of carbon dioxide (CO_2) since the industrial revolution. In 2023, it reached a new peak of 425 parts per million (ppm), and this trend is only going to become worse in the coming decades. Potential candidates for minimizing the environmental effects of CO_2 emissions are porous polymer polymers (POPs), which are recognized for their exceptional stability and well-developed porosity. In this research, two newly synthesized POPs named PP7 and PP8 are prepared using triptycene and tetra-2-pyridinylpyrazine via Friedel-Crafts alkylation with and without dimethoxymethane, respectively. To confirm the synthesis, NMR, FTIR and XRD studies were conducted, and it was also noted that the polymers are thermally stable up to 300 ºC. The BET surface was also determined, and the values are 1027 and 699 m^2/g as shown in Figure 1a. The CO_2, CH_4, N_2 and H_2 gas adsorption studies were performed at 273 K and 298 K and PP7 performed well at both temperatures for all gases. Specifically, the CO_2 uptake values were 2.62 and 2.18 mmol/g (Figure 1b) and H_2 values are 5.10 and 4.59 mmol/g for PP7 and PP8 at 273K, respectively. The isosteric heat of adsorption (Q_{st}) was calculated using Clausius-Clapeyron equation and the results provided the higher values for CO_2 as compared to CH_4 and N_2 for PP7 and PP8. Based on these results, it can be elucidated that the prepared polymers are the potential materials for CO_2 capture and clean energy applications.

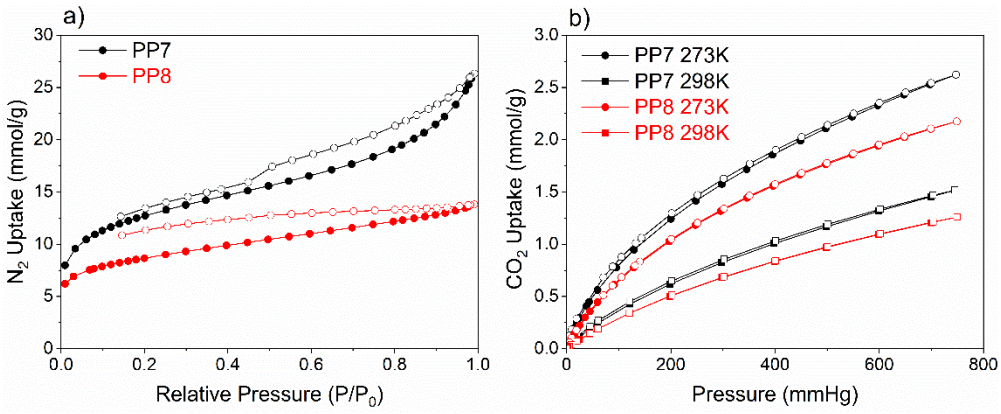

Fig. 1. PP7 and PP8 data of a) N_2 adsorption and desorption at 77K for surface area b) CO_2 adsorption data at 273K and 298K

Keywords: Polymerization, porous organic polymers, CO_2 capture, adsorption isotherms, environmental applications.

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EES - D3 - P50

Assessment of some organochlorine pesticides and toxic heavy metals in the road dust from a metropolitan city in Nigeria: Akure as a case study

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Environmental pollutants are on the rise due to several anthropogenic activities in cities across the globe. Organochlorine (OC) pesticides are one of such pollutants used for various purposes. Heavy metals on the other hand have been reported for their numerous toxicities. Samples were taken from seven different locations and analysed using standard methods. The following OC pesticides congeners - α-HCH, β-HCH, γ-HCH (Lindane), and δ-HCH, popularly called the hexachlorocyclohexane were analysed. They are in the following range: BDL – 2.272 µg/kg for α-HCH, BDL – 10.080 µg/kg for β-HCH, 4.872 – 31.834 µg/kg for γ-Lindane, and BDL for δ-HCH. Lindane was detected from all the sampling locations with significant concentrations. The highest is from the sampling location 7 (SL 7) while the least is from the sampling location 5 (SL 5). The highest ∑ HCHs is from the sampling location 7 (SL 7) (41.914 µg/kg) while the least is from the sampling location 3 (SL 3) (7.146 µg/kg). The order of increase of the HCHs with the locations is SL 7 > SL 3 > SL 2 > SL 4 > SL 6 > SL 5 > SL 1. Source identification showed fresh, industrial and historical usage from some of the sampling locations. The concentrations of the selected toxic heavy (THM) metals are in the following range (mg/kg): Pb (0.49±0.00-0.72±0.00), Cd (0.15±0.00 - 0.32±0.00), As (0.06±0.01 - 0.37±0.00), Cu (1.35±0.00 – 3.24±0.00), Cr (1.70±0.00 - 3.58±0.00), Co (0.05±0.01 - 0.22±0.01), and Ni (0.43±0.05 - 0.92±0.00). The degree of their concentrations in the order of Co > As > Cd > Pb > Ni > Cu > Cr. The sources of heavy metals are similar with Pb having a different source. Lindane is predominant in road dust samples which can cause several environmental and human health problems including the THMs.

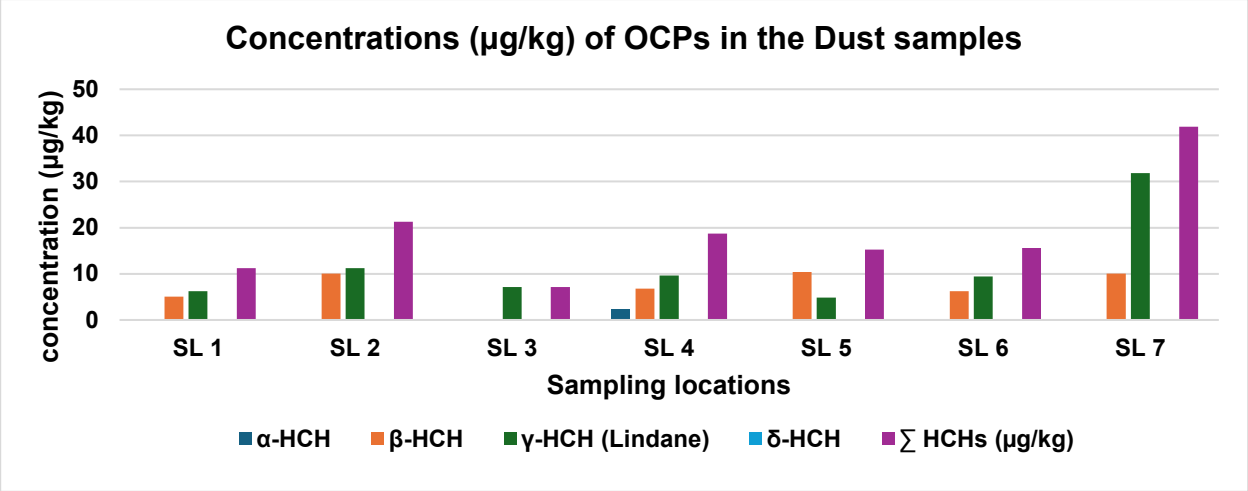

Fig.1. OCPs concentration (µg/kg) in the road dust samples from the locations

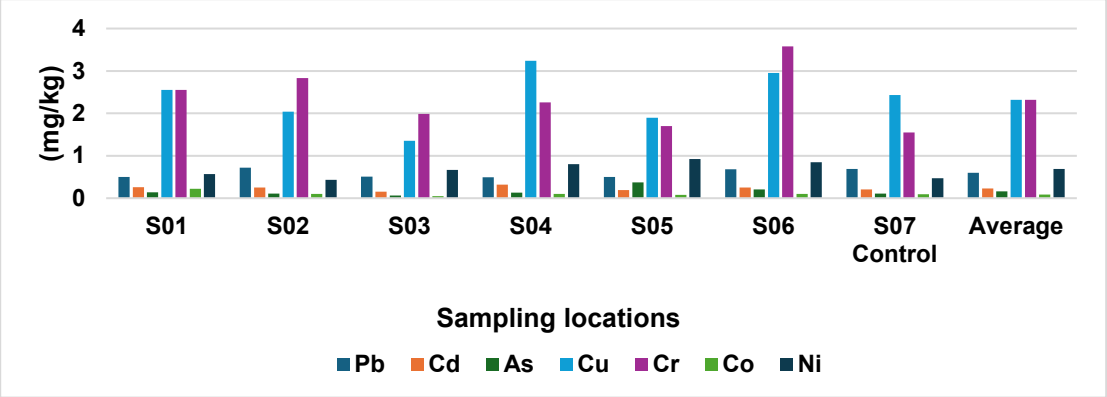

Fig. 2. Chart showing heavy metal concentrations across all the sampling locations

Key words: Toxic heavy metals, pesticides, HCHs, Road Dust, Lindane, health assessment.

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EES - D3 - P60

Removal of nitrogenous heteroaromatic compounds from gasoline using the deep eutectic solvent diethanolamine: glycerol

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Among the gases that harm the environment and aquatic ecosystems are nitrogen oxides (NO_X), which are partly responsible for the greenhouse effect and acid rain. Their sources are numerous, but the primary source is the combustion of nitrogen compounds contained in hydrocarbons using in industry, transportation and domestic heating. These compounds end up in fuels (gasoline, diesel, kerosene, and heavy fuel oil) used in everyday human life. In recent years, a family of deep eutectic solvents (DESs) has been emerged. Thanks to their environmentally friendly properties, these solvents are classified as green solvents. These solvents are formed by mixing a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), resulting in a liquid phase with a melting point lower than that of its components in their pure state[1]. In this work, the DES, Diethanolamine: glycerol [1:2], was prepared and used to remove pyridine and quinoline from n-heptane, using the liquid-liquid extraction technical. N-heptane is considered as a model molecule for gasoline. To this end, two liquid-liquid equilibrium (LLE) systems {n-heptane + pyridine/quinoline + DES} were experimentally measured at 298.15 K and 1 atm. The obtained results are show in Fig. 1, the two ternary diagrams are category I type according to the classification of Sorensen et al.[2], with partial miscibility between n-heptane and DES and complete miscibility between the nitrogen compounds with n-heptane and DES. The experimental LLE values were correlated using the NRTL method[3] and the COSMO-RS model[4]. The NRTL correlation results are in very good agreement with the experimental values for two systems. In contrast, the COSMO-RS model results, while qualitatively consistent with the experimental results, show a more or less significant quantitative discrepancy between the two mixtures. In conclusion, the DES (Diethanolamine: glycerol) can be considered as a promising extracting agent for nitrogen compounds from gasoline.

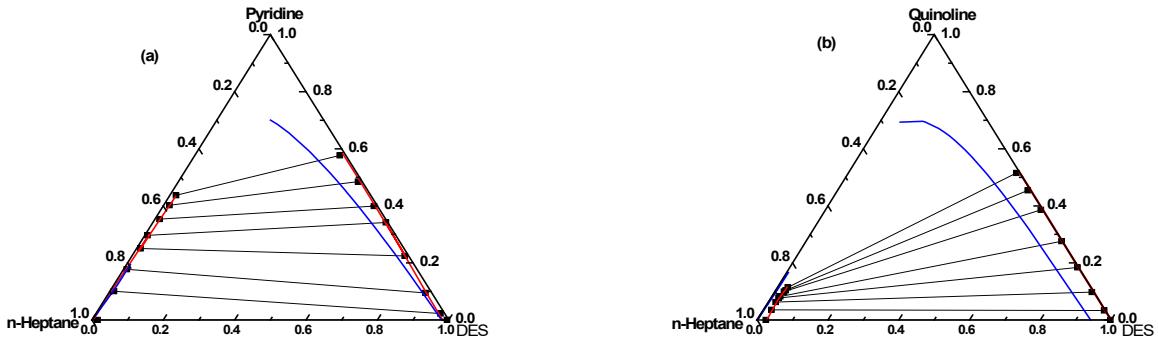

Fig. 1. Ternary LLE diagrams in molar fractions for systems: (a) (n-heptane + pyridine + DES), (b) (n-heptane + quinoline + DES), (–■–) Experimental measured tie lines; (–), NRTL binodal curve calculated; (–), COSMO-RS binodal curve calculated.

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Innovative Materials (IM)

IM - D3 - P01
Multifunctional degradable titanium coatings for osteointegrative and antimicrobial surfaces

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The rational design of multifunctional surface coatings for titanium implants requires precise control over composition, interfacial chemistry, and degradation behavior in biologically relevant environments. Recent advances in hybrid materials chemistry emphasize the importance of combining organic and inorganic building blocks to achieve synergistic functionality through controlled interfacial interactions [1-3]. In this contribution, we report a degradable hybrid composite coating deposited on titanium substrates via a dip-coating strategy, integrating biopolymeric and mineral phases to achieve enhanced bioactivity and antimicrobial performance.
The coating system is based on a multilayer composite architecture that combines collagen and nano-hydroxyapatite (nHA) as an inner bioactive phase with an outer chitosan-based biodegradable matrix incorporating gold-doped zinc oxide quantum dots (ZnO: Au QDs) and nystatin [4,5]. From a chemical standpoint, collagen and nHA form a hybrid interface stabilized by hydrogen bonding, electrostatic interactions, and calcium–phosphate coordination, closely resembling mineralized extracellular matrices. Chitosan provides a cationic polymer network capable of interacting with both the hybrid layer and the embedded functional species through non-covalent interactions, including ionic pairing and hydrogen bonding. These interactions play a key role in controlling coating cohesion, stability, and degradation behavior [6].
The dip-coating approach enables precise control over layer composition and thickness, while crosslinking reactions ensure sufficient coating integrity without compromising biodegradability. Chemical and structural characterization using complementary spectroscopic and microscopic techniques provides insight into hybrid interfacial interactions, which govern coating stability, degradation kinetics, and the release behavior of active components. The degradable nature of the composite allows gradual exposure of the bioactive phase and controlled release of antimicrobial and antifungal agents, primarily driven by matrix erosion and interfacial chemistry rather than bulk dissolution.
Overall, this work highlights how rational hybrid materials chemistry enables the design of advanced multifunctional coatings that bridge fundamental interface engineering with application-driven requirements for next-generation titanium-based implant surfaces.

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IM - D3 - P02

Development of 2D nanosheets of lanthanide-based metal organic frameworks for developing a super-hydrophilic and super-oleophobic (underwater) selective layer on a ceramic support for separation of surfactant-stabilized oil-in-water emulsion

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The current study aimed to develop an active layer composed solely of metal-organic frameworks for the efficient separation of oil-in-water emulsions. This was achieved by in situ growth of 2D nanosheets of a Ln-based metal-organic framework via solvothermal synthesis on a ceramic alumina disc. As a result, a continuous, defect-free active layer was formed on the ceramic alumina support. The resultant membrane, named as Ln-5-NH_2-IPA MOF, was studied for the separation of oil-in-water emulsion. The ultimate goal of the current study was to reduce the time and temperature required to synthesize 2D MOF sheets with a stable, active layer that can be tested under crossflow filtration conditions. The thickness of the 2D MOF nanosheets was found to be 1.8 nm on average, as observed in transmission electron microscopy. The *in-situ* growth of the 2D MOFs resulted in a dense coating on the ceramic support, resembling the leaves of densely growing trees in a forest. Owing to the dense growth of the 2D MOF on the ceramic support, the Ln-5-NH_2-IPA MOF membrane showed a high separation efficiency of >99% for the surfactant-stabilized 100 ppm crude oil-in-water emulsion during separation studies. Moreover, the membranes showed a permeance of 147.9 L m^{-2} h^{-1} bar^{-1} while using a crude oil-in-water emulsion. The membrane maintained stable performance, especially in separation efficiency, for 660 minutes, whereas its performance declined, with the normalized flux decreasing to 0.20 over 360 minutes. However, the membrane regained its flux following the cleaning cycle.

The authors are highly grateful for the support provided for conducting the current study. The current study was conducted at the Interdisciplinary Research Center for Membranes and Water Security at King Fahd University of Petroleum and Minerals, KSA.

IM - D3 - P03

Development of spherical Mg-Al silicate composites for simplified purification and enhanced filtration of C.A.S.E. polyols

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Conventional sequential purification using magnesium and aluminum silicates for C.A.S.E. polyols is often challenged by process complexity and limited filtration efficiency. To address these limitations, this study developed a spherical Mg-Al silicate composite enabling a simplified, single-step purification process.

The optimized composite exhibited an average particle size of 94.60 ㎛ and a specific surface area of 514.51 m^2/g. Upon applying polyol purification, it achieved a 33.33% reduction in the CPR (reaching 30), thereby markedly improving reaction stability, while simultaneously decreasing filtration time by 52.66% (to 71 s).
These results demonstrate that the developed Mg-Al silicate composite substantially enhances overall process efficiency and offers a promising approach for the simplification and potential automation of high-purity polyol production.

IM - D3 - P04
Ultrathin macroporous substrates for near-field microscopy on free-standing membranes

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Pore-spanning membranes (PSMs) are unsupported membrane segments suspended over a macroporous substrate for investigating the physical and functional properties of lipid bilayers under well-controlled conditions [1, 2, 3]. Conventional PSMs are typically optimized for far-field fluorescence microscopy, which limits spatial resolution and signal quality [4]. Integrating the PSM concept with advanced imaging techniques, such as optical super-resolution or near-field microscopy, has remained challenging. To this end, smooth macroporous substrates with nanoscale thickness and adequate mechanical stability are required. The macropores should have diameters of a few hundred nanometers, while the interpore spacing must be sufficiently large to allow individual macropores to be addressed by diffraction-limited microscopy and to enable the tethering of membranes on the macroporous substrates. Here, we report the use of porous alumina anodized with etidronic acid solutions [4] as a template for the fabrication of ultrathin macroporous gold foils that meet these stringent requirements. The undersides of the alumina templates were exposed by wet etching, followed by reactive ion etching to open the alumina pore bottoms. This procedure yielded a smooth macroporous surface suitable for gold deposition. After non-destructive detachment, unsupported ultrathin gold foils—containing holes corresponding to the initial alumina pore positions—were obtained and subsequently transferred onto microscope slides. By fine-tuning pore diameters and interpore spacing, lipid membranes can be suspended over the macroporous openings, ensuring minimal background, efficient signal transmission, and compatibility with high-intensity illumination. Our goal is to integrate PSMs with state-of-the-art super-resolution and near-field microscopy techniques, thus enabling nanoscale investigations of membrane organization and dynamics in unsupported membrane segments.

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IM - D3 - P05
Carbon dots from renewable biomass precursors: Processing parameters and optical response

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Biomass-derived carbon dots (CDs) constitute a heterogeneous family of nanostructured materials whose optical properties depend strongly on precursor composition and processing conditions[1,2]. This contribution addressed the preparation of CDs by bottom-up methods from selected waste streams, specifically hemicellulose and lignin from commercial sources and from residues such as almond shells and pig dry manure. The diversity of these feedstocks provided a basis for examining how the chemical composition influenced the characteristics of the resulting particles.
CDs were prepared by hydrothermal synthesis, and several experimental parameters were explored, including the pre-treatment of raw materials, the choice of solvent system, reaction temperature and duration, precursor concentration, and the application of simple pretreatments to the raw biomass. The objective was to determine how these variables affected the formation process and the optical response of the products. Standard physicochemical characterization techniques were employed to obtain information on particle size, surface properties, and functionality, as well as photoluminescence features.
As a potential application, the response of the synthesised CDs to temperature was examined to assess their suitability as luminescent probes. Changes in emission intensity and spectral profile under controlled heating–cooling cycles were used as preliminary indicators of sensitivity and reversibility. The work sought to contribute experimental information on the conversion of heterogeneous biogenic precursors into carbon-based nanomaterials and on the practical constraints associated with their reproducible preparation.

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IM - D3 - P06
Imination of aminocaprolactam with bio-based aldehydes to produce bio-based polyamides

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A significant part of the development of modern society has relied on the use of fossil resources, both in the past and present. However, the growing global demand for carbon-based materials cannot be met by these finite reserves. Consequently, biomass has evolved as an important renewable carbon source and moved in the focus of current research. Trough the fermentation of sugars, the amino acid lysine can be produced in large quantities. Owing to its multifunctionality, featuring one carboxylic acid group, as well as two amino groups, lysine represents a promising bio-based platform chemical for the synthesis of value-added products.[1] The natural occurring homopolymer of lysine, ε-polylysine, is produced through fermentation but is limited to a low molecular weight range. Accessing high molecular weight ε-polylysine therefore requires a chemical approach. Conventionally, this involves cyclisation of lysine, protection of the α-amino group, polymerisation, and subsequent deprotection. Eliminating the protection step would significantly enhance the efficiency and sustainability of the process.[2]
The aim of this study was to develop bio-based monomers suitable for the production of ε-polylysine, while avoiding the protection step. Therefore, methylvanillin was employed as a bio-based aldehyde to form an imine with cyclised lysine. The reaction was carried out in methanol without the use of any additives. Reaction conditions were optimised with respect to temperature, time, concentration and aldehyde excess using a Bayesian optimisation. Highly selective conditions were identified, resulting in an imine yield of 91%. Furthermore, the substrate scope was extended to six additional bio-based aldehydes. In all cases, yields between 80 and 90% were achieved, demonstrating the robustness and versatility of the developed approach.

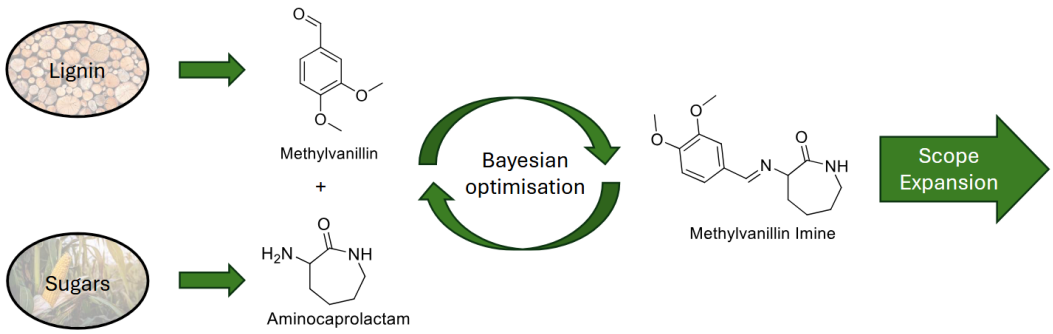

Fig. 1. Bayesian optimisation of aminocaprolactam imination and substrate scope.

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IM - D3 - P07

Polymerization of malononitrile dimer: A new route for construction of nitrogen-rich polytriazines with functional properties

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The search for new polymerization paths is an inevitable challenge in materials science, mainly with the advantages of simple operation, mild conditions, high efficiency, low cost, environmental benefits, reliability, and scalability. After many decades of exploring the chemistry of the C-C double bond, recently polymerizations based on triple bond building blocks have taken a clear lead role. Remarkable progress has been made in those where alkynes are used, however nitrile monomers have been less studied.
In this context, the thermally induced polymerization of amino-nitrile monomers, like the diaminomaleonitrile (DAMN), is becoming a valuable alternative to conventional polymerization methods, meeting the requirements argued above. Substantial advancements have been conducted by our group, starting with research on DAMN, which has been successfully polymerized thermally, both in solution and in bulk, yielding materials with interesting optoelectronic properties and promising applications.[1,2] In this same line, we have also focused on the bulk liquid thermal polymerization of aminomalononitrile.[3] The easy, quick, and highly efficient polymerization of these dinitrile compounds motivated the exploration of new multinitrile monomers, such as the malononitrile dimer, 2-amino-1,1,3-tricyanopropene (ATCP). Thus, a recent work revealed ATCP as a promising amino-nitrile monomer for the straightforward, one-pot synthesis of C=N conjugated organic materials featuring triazine linkages. DSC confirmed the successful bulk polymerization of ATCP, which proceeds upon melting and is initiated at relatively low temperatures without the need for solvents, catalysts, or initiators. The kinetic study carried out demonstrated the autocatalytic character and corroborated that these thermally induced reactions are extremely fast in a molten state. In addition, a preliminary structural characterization by spectroscopy supported the formation of triazine-based polymeric networks.[4]
These precedents encouraged us to explore the bulk thermal polymerization of ATCP at the preparative scale, and the structural characteristics of these ATCP-based polymers and their properties are discussed.

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IM - D3 - P08

Biogenic synthesis of zinc oxide nanostructures using Adansonia digitata peel extract for sildenafil degradation and photocatalytic performance

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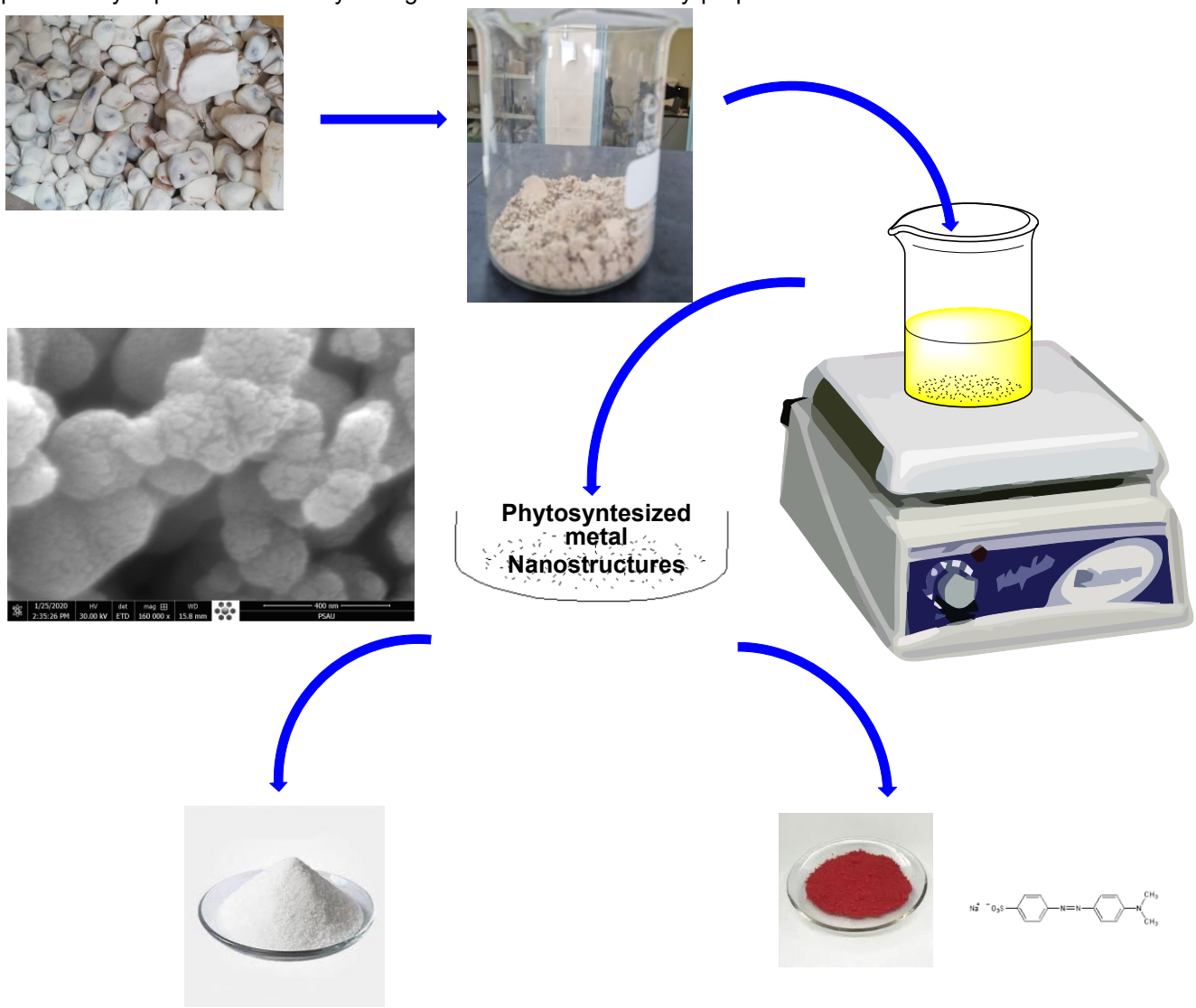
Adansonia digitata plant usually used as source of food in many African countries. it contains many active compounds. In addition, its leaves and fruit extract was used as green source to prepare versatile metallic nanoparticles.[1] *Adansonia digitata* peel have been selected as a green route to the preparation of stable and shape-controlled zinc oxide nanostructures. Herein, an ecofriendly process based on using the water extract of *Adansonia digitata* peel to synthesize of ZnO nanoparticles[2]. The characterization of calcined zinc nanostructures, were performed using various physicochemical technics such as, Fourier-transform infrared spectroscopy, Raman, x-ray diffraction, Scanning electron microscope and X-ray photoelectron spectroscopy. Analytical characterisation technics used confirm the preparation of the targeted stable nanostructure. The photocatalytic sildenafil degradation of the green synthesized metal (Zn) nanostructures was assessed. Overall, the prepared zinc nanoparticles showed good efficacy towards degradation of tested drug. In addition, photocatalytic performance of dyes degradation of the ecofriendly-prepared nanostructures was also tested[3,4].



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IM - D3 - P09
Self-assembly of an amphiphilic copolymer and its potential as drug delivery systems

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The design of advanced drug delivery systems has gained increasing interest in recent years in order to achieve the safe, efficient, and dose-controlled delivery of therapeutic agents to their intended targets. Among these systems, polymeric micelles derived from amphiphilic block copolymers have emerged as attractive carriers due to their ability to solubilize poorly water-soluble drugs and to provide controlled and prolonged release behaviors [1,2].
In the current study, a novel amphiphilic block copolymer, poly[(ethylene glycol) methyl ether methacrylate]-*b*-poly[(glycerol carbonate methacrylate)-*co*-(diisopropylamino)ethyl methacrylate] (PEGMEMA-*b*-P(GCMA-*co*-DPA)), was synthesized using reversible addition–fragmentation chain-transfer polymerization. The chemical composition and molecular characteristics of the copolymer were determined with ^{1}H NMR spectroscopy and gel permeation chromatography. At pH 7.4, the copolymer spontaneously self-assembled into polymeric micelles with an average hydrodynamic diameter of 20.1 nm. The structural features and morphology of the micelles were further investigated by ^{1}H NMR spectroscopy and transmission electron microscopy. Dipyridamole was employed as a model hydrophobic drug and efficiently encapsulated within the micellar core. The encapsulation efficiency and drug loading capacity of the micelles were quantitatively evaluated by UV–Vis spectroscopy.
In vitro drug release experiments conducted at pH 7.4 demonstrated controlled release profile. Overall, the findings indicate that PEGMEMA-*b*-P(GCMA-*co*-DPA) micelles represent a promising and adaptable carrier system for the delivery of hydrophobic therapeutic agents.

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IM - D3 – P10
Design of new PEG-silanized fillers inspired by talc-like structures

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Polymer–clay composites are well known for their enhanced mechanical and thermal properties, provided that the inorganic filler is homogeneously dispersed within the polymer matrix. Achieving such dispersion, however, remains challenging, particularly due to limited compatibility between polymers and pre-formed clay minerals. In this work, we investigate a fundamentally different approach, consisting of generating clay-like fillers in situ using silanized polymers as the silicon source. Beyond improving interfacial compatibility, this strategy also avoids the direct handling of nanoparticles, thereby reducing potential health risks.
Poly(ethylene glycol) methyl ether (mPEG) was functionalized with (3-isocyanatopropyl)triethoxysilane, yielding silane-terminated polymers with high functionalization efficiencies, exceeding 90%. These precursors were reacted with magnesium nitrate in ethanolic solution under basic conditions. mPEGs with molar masses ranging from 350 to 1900 g mol^{-1} were investigated, both alone and in combination with conventional silicon sources, tetraethyl orthosilicate and (3-aminopropyl)triethoxysilane.
When functionalized mPEG was used as the sole silicon source, the synthesis yields remained low, between 8 and 22 wt%. In contrast, combining functionalized mPEG with tetra or trialkoxysilane led to a threefold increase in yield, indicating enhanced network formation. Structural characterization by X-ray diffraction and FTIR spectroscopy revealed the formation of layered crystalline materials containing both Si–O and Mg–O bonds. However, solid-state 1H–29Si CPMAS NMR showed that silicon condensation was incomplete, with silicon predominantly present in T1 and T2 environments. SEM-EDX analysis further revealed Mg/Si molar ratios exceeding that of ideal talc.
Taken together, these results indicate that the synthesized materials more closely resemble functionalized brucite-like sheets rather than true talc analogues.[1] Nonetheless, this work establishes a viable route toward the in situ formation of layered organic–inorganic hybrids and provides a promising basis for the development of polymer–clay nanocomposites with improved filler dispersion

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IM - D3 – P11

Mass spectrometry–driven evaluation of antioxidant thermoplastic polyurethane films for waste cooking oil storage

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The stabilization and valorization of waste cooking oil (WCO) rely on storage solutions that can slow down oxidation and preserve the oil quality over time [1,2]. In this work, thermoplastic polyurethane (TPU) films containing α-tocopherol were developed as active materials for WCO storage. Their performances were evaluated using a combination of physicochemical and mass spectrometry-based analysis.

α-Tocopherol was selected as an active component as it combines strong antioxidant activity with a high affinity for lipid-rich systems, making it particularly suitable for interaction with waste cooking oil. TPU films with α-tocopherol between 5 and 20 wt% were prepared and characterized in terms of optical, thermal, mechanical, and barrier properties. The addition of the antioxidant improved UV protection, increased film flexibility, and reduced water vapor permeability, while preserving the mechanical strength and thermal stability required for real storage conditions.

Mass spectrometry played a central role in understanding how these materials work. LC–ESI–MS/MS was used to follow the controlled release of α-tocopherol into a lipid simulant, showing a sustained diffusion over time. Surface-sensitive analyses further indicated that the active compound can migrate to and from the film surface without causing polymer degradation.

To assess real performance, waste cooking oil was stored in contact with the TPU films and its chemical stability was monitored over time. MALDI–MS allowed direct molecular profiling of triacylglycerols, revealing that oils stored with TPU–α-tocopherol films retained a molecular composition closer to that of fresh oil after 90 days. In contrast, untreated samples showed clear signs of oxidation and degradation.

Overall, this study shows that TPU films incorporating α-tocopherol offer an effective and practical solution for extending the stability of waste cooking oil. The consistent use of mass spectrometry throughout the study highlights its value as a powerful tool for linking material design to molecular-level performance.

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IM - D3 – P12

A multifunctional nitrogen-doped magnetic graphene oxide nanocomposite prepared by one-step microwave-assisted synthesis

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This work reports the synthesis and characterization of a multifunctional nanocomposite based on magnetite-functionalized graphene oxide (mNGO), obtained through a one-step microwave-assisted hydrothermal route. The proposed strategy was designed to provide a rapid and controllable method for producing hybrid materials with integrated magnetic and photoactive properties. Graphene oxide (GO), prepared using the modified Hummers method, was used as the precursor matrix. Ethylene glycol was utilized as a solvent, dispersing medium, and mild reducing agent, while urea provided the nitrogen source. Sodium acetate was found to play a pivotal role in maintaining pH balance and facilitating iron oxide coprecipitation, while PEG-6000 functioned as a steric stabilizer. The formation of magnetite was accomplished through the utilization of $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$, in conjunction with microwave heating at an elevated temperature of 180°C for a duration of 30 minutes. The resulting material exhibited a homogeneous black coloration and a pronounced magnetic response, indicating a successful functionalization process. Scanning electron microscopy revealed the presence of spherical nanoparticles distributed over graphene oxide (GO) sheets, with diameters ranging from 20 to 50 nanometers. X-ray diffraction was used to confirm the disappearance of the characteristic GO peak and the emergence of reflections assigned to the spinel phase of magnetite. The FT-IR spectra indicated a partial reduction of GO, Fe–O vibrations, and nitrogen-containing groups, thereby supporting both magnetic functionalization and heteroatomic doping. Raman spectroscopy revealed a progressive increase in the I(D)/I(G) ratio, suggesting an escalating degree of structural disorder following successive modifications. Zeta potential values at pH 6.8 indicated moderate colloidal stability and a positively charged surface. In summary, the implementation of this one-step approach resulted in the successful development of a hybrid multifunctional material that exhibits considerable promise for utilization in diagnostic, imaging, and photoactivated applications.

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IM - D3 – P13

Dual crosslinked printable chitosan/PEG/γ-cyclodextrin hydrogels with tunable rheological properties

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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 (γCD) with different crosslinking mechanisms were developed. The hydrogel systems were prepared using covalent crosslinking approaches based on amino-yne "click" reactions with PEG-DA and divinyl sulfone (DVS) as crosslinker, and combinations of these two systems were also investigated.[1] In addition to primary covalent bonds, hydrogen bonds formed through the hydroxyl groups of γCD provided secondary physical interactions, contributing to the structural integrity of the system. Thanks to this double crosslinking approach, flow was achieved by breaking physical bonds during printing, while covalent bonds and recovered hydrogen bonds maintained the stability of the structure after printing. Rheological analyses showed that the developed hydrogel systems exhibited a self-supporting structure with storage modulus in the range of 10^3–10^4 Pa and tanδ<1 values as shown in **Table 1**. Furthermore, it was determined that the systems exhibited shear thinning and thixotropic behavior. SEM analyses revealed that the hydrogels have a porous and interconnected internal structure. The findings indicate that the developed hydrogel systems are promising candidates for tissue engineering and biomedical applications.

Table 1. Rheological results of hydrogels.

Gel	η (Pa.s)	Max G' (Pa)	tanδ	Gelation T (℃)	90% Recovery (s)
CPGT1	516.8	3165.6	0.2	27.4	10
CPGT2	792.8	4812.9	0.3	28.5	25
CPGT3	1600	9790.4	0.2	20.0	5
CPdGD3	731.7	4533.9	0.2	32.7	9
CPdGD4	1349.2	8208.1	0.3	27.4	38
CPdGD5	250.4	1553.3	0.2	27.4	10

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IM - D3 – P14
Electrosynthesis of molecular cluster assembly materials with hierarchical porosity

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We report an electrochemically mediated assembly strategy that couples N-heterocyclic carbene (NHC)–protected tetrairidium clusters into one-dimensional oligomeric chains via direct metal–metal bonds, yielding self-assembled extended architectures with lengths of several nanometres. The hallmark is synthesis of these architectures with the molecular integrity of the individual clusters preserved. We demonstrate this approach across different cluster platforms starting with calix[4]arene-phosphine-protected triruthenium clusters, which are selected for their known propensity toward ring-opening reactions.[1] This concept is generalized with the attachment of a calix[4]arene-functionalized NHC ligand to a tetrairidium core[2,3] produces a hierarchically porous material. We demonstrate that the resulting molecular cluster assembled materials (MCAMs) exhibit emergent macroscopic properties that are highly dependent on the nature of the organic ligand, featuring interconnected pores with dimensions of several hundred nanometres and ultrathin walls down to 5 nm. Notably, the walls themselves are nanoporous, leading to a multiscale porous architecture that bridges molecular, nano-, and mesoscale organization. This approach provides a versatile bottom-up route to hybrid organic–metal materials from discrete molecular clusters, opening new opportunities for designing functional porous materials with tuneable structural and chemical properties relevant to catalysis and other functions relying on high exposed surface areas.

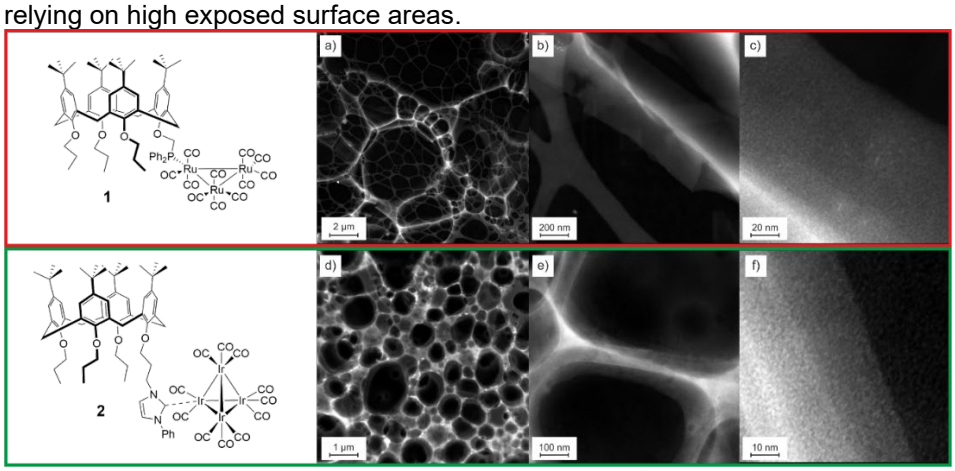

Fig. 1. Starting triruthenium cluster phosphine-complex 1 and starting tetrairidium cluster NHC-complex 2 with HAADF-STEM images with different magnifications of the MCAMs consisting of 1-red (a-b), and 2-red (d-f).

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IM - D3 – P15
Twist and resist: Stability and chiroptical enhancement in chiral hybrid perovskites

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Novel materials that are able to discriminate between left- and right circularly polarized light are in high demand for application in fields such as chiral optoelectronic technology and spintronics. With their unique blend of organic and inorganic components, 2D chiral hybrid perovskites (CHPs) have received increased interest due to their potential to be incorporated as active layer in CPL-LEDs, spin-LEDs and highly sensitive CD detectors. So far, the organic cations are equipped with an asymmetrical carbon atom to induce asymmetrical distortions to the inorganic framework (Fig .1), forming a semiconductor that is sensitive to the polarization of light. The hybrid character of this chiral semiconductor family offers a large degree of freedom regarding bandgap and energy alignment tuning. Nevertheless, CHPs are accompanied by a lower environmental stability than their achiral counterparts due to induced structural distortions by the chiral cations. This work focuses on increasing the intrinsic stability of 2D CHPs while maintaining chiroptoelectronic properties through tailored organic cation design.

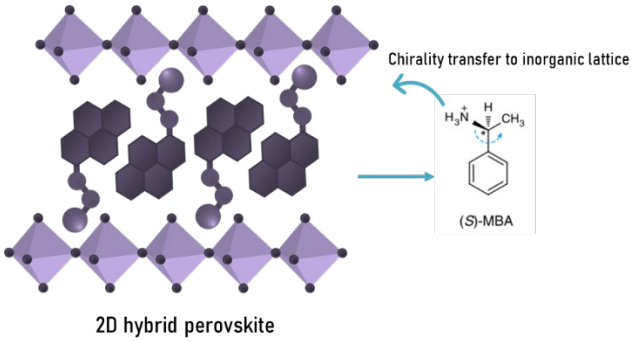

Fig.1. Representation of a 2D CHP

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