3rd Bilateral Workshop Portugal – Slovenia

WORKSHOP (Bio)materials and Processes for Circular Economy

BOOK OF ABSTRACTS

University of Aveiro, Portugal

September 4–5, 2025

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3rd Bilateral Workshop Portugal – Slovenia

Message from the chairs:

This series of workshops was launched in 2022 with the aim of fostering close collaboration between the research groups from Portugal and Slovenia. It started with the research groups from CERES, University of Coimbra, and the National Institute of Chemistry (NIC). In the second edition, it expanded to welcome researchers from a broader range of institutions and disciplines, mainly from Portugal and Slovenia, but also with a wide international contribution, laying the groundwork for an international dialogue.

In this third edition, we are pleased to see the workshop consolidating even more its role as a bridge between Portugal and Slovenia, now being organized by research groups from CICECO- Aveiro Institute of Materials, University of Aveiro (Portugal) and NIC (Slovenia). The workshop has strengthened its national profiles through the participation of multiple Portuguese universities and a relevant number of researchers from NIC. At the same time, we are honoured to host invited speakers from other countries, further enriching the scientific discussion and future perspectives.

In a time when circular solutions are more urgent than ever, this workshop provides a platform to share ideas, present new results, and exchange experiences across disciplines. What began as a bilateral initiative has grown into a space for wider dialogue on biomass valorization, sustainable (bio)materials, green processes, and advanced tools for the circular economy.

By bringing together expertise that ranges from experimental chemistry and materials engineering to computational modelling and bioprocess optimization, the workshop fosters a multidisciplinary environment where different approaches complement one another. We believe that this diversity of perspectives is key to driving innovation and to developing practical solutions for today's sustainability challenges.

We warmly welcome all participants and thank you for contributing to this collaborative effort. We hope this workshop will not only showcase excellent science but also inspire groundbreaking ideas and lasting collaborations.

Workshop Co-chairs:

- Mara G. Freire (University of Aveiro, Portugal)
- Filipa A. Vicente (Kemijski Institut, Slovenia)

Organizing Committee:

- Filipa A. Vicente
- João A. P. Coutinho
- Jorge F. B. Pereira
- Mara G. Freire
- Márcia Neves

Acknowledgements:

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Plenary session

Nature's Solution to Forever Chemicals: Natural Deep Eutectic Solvents for Circular PFAS Remediation

Santiago Aparizio Martinez[1]

[1]Department of Chemistry – ICCRAM, University of Burgos, 09001 Burgos – Spain

Per- and polyfluoroalkyl substances (PFAS) represent one of the most pressing environmental challenges of our time, contaminating drinking water, wastewater, industrial effluents, and natural water bodies worldwide. Their exceptional persistence and bioaccumulation properties have earned them the designation "forever chemicals," while evolving regulations demand urgent, cost-effective remediation solutions.

This talk presents a comprehensive approach to PFAS removal using natural deep eutectic solvents (NADES) as sustainable alternatives to conventional treatment technologies. Current state-of-the-art methods, including activated carbon adsorption, ion exchange, and advanced oxidation processes, face significant limitations in terms of cost, energy requirements, and complete mineralization. The technoeconomic analysis reveals critical gaps that NADES can address within circular economy frameworks.

Through multiscale simulation approaches, it is demonstrated the rational design of NADES tailored for selective PFAS extraction across diverse water matrices. Molecular dynamics simulations and density functional theory calculations guide the selection of bio-derived components, optimizing solvent-PFAS interactions while maintaining environmental compatibility. Laboratory-scale validation confirms exceptional removal efficiencies for both short- and long-chain PFAS compounds, with regeneration protocols enabling solvent reuse.

The technoeconomic feasibility study for scaling up reveals promising pathways for Technology Readiness Level advancement, with potential for industrial implementation. Life cycle assessment confirms the environmental benefits of NADES-based processes compared to conventional methods, aligning with circular economy principles through bio-based feedstock utilization and closed-loop operation.

Future directions include pilot-scale demonstrations, regulatory pathway development, and integration with existing water treatment infrastructure. This work establishes NADES as a transformative technology for sustainable PFAS remediation, offering nature-inspired solutions for one of the most challenging environmental problems of the 21st century.

Keynote sessions

Cellulose Beads as Sustainable Tools for Water Remediation

Carla Vilela[1]

[1]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

Cellulose is the most abundant natural polymer and, as a result of its renewability, abundance, low cost and fascinating structure and properties, is being investigated to produce materials for water remediation.[1] Although this polysaccharide is mostly used in the form of fibers and nanofibers, it can also be utilized in the form of particles at the micro and nanoscales,[2] exhibiting large surface area and abundant surface hydroxyl groups that enable a variety of physical and chemical modifications. Thus, the present communication will highlight cellulose-based microparticles, specifically hybrid beads of cellulose functionalized with inorganic nanoparticles, as innovative tools for water treatment. These hybrid beads were engineered to possess bioactive and functional properties, including antibacterial activity, catalytic propulsion, magnetic responsiveness and oxidizing power. The cellulose beads were fabricated via dissolution of wood pulp fibers in an organic electrolyte solution followed by regeneration in water, and functionalization with inorganic nanoparticles. The resulting hybrid beads exhibited the envisioned bioactive properties and showed significant potential in removing organic pollutants. This approach offers a promising avenue for advanced water treatment tools, featuring the added benefit of reusability over several cycles.

Keywords: Cellulose, Inorganic nanoparticles, Biopolymeric hybrid beads, Water remediation

Acknowledgments

This work was developed within the scope of the project CICECO – Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), and project Cell4Janus (PTDC/BII-BIO/1901/2021, DOI 10.54499/PTDC/BII-BIO/1901/2021), financed by national funds through the FCT/MCTES(PIDDAC). FCT is also acknowledged for the research contract to C.V. (DOI 10.54499/2021.01571.CEECIND/CP1659/CT0024).

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Aqueous Two-Phase Systems: Advanced Tools for Integration of Circular Processes

Jorge Pereira[1]

[1] CERES, Department of Chemical Engineering, Faculty of Sciences and Technology of the University of Coimbra, Coimbra, Portugal

Aqueous Two-Phase Systems (ATPS), also widely known as Aqueous Biphasic Systems (ABS), have been extensively applied as advanced separation and purification methods, particularly for the recovery of bio-based products.[1] These liquid-liquid extraction take advantage of their water-rich composition and low interfacial tension to create unique immiscible aqueous environments, where biocompatibility and versatility are achieved through the careful selection of phase-forming components (*e.g.*, polymers, salts, ionic liquids, short alkyl chain alcohols, sugars).[1]

This talk will provide a brief overview of the research conducted in my laboratory over the past several years, with a particular focus on case studies where ATPS were employed to enhance the integration of downstream processing operations, highlighting their potential role in fully circular (bio)processes.

The presentation will begin with fundamental principles for selecting appropriate ATPS formulations for specific applications,[1,2] followed by examples of applied processes in which ATPS were successfully integrated into Centrifugal Partition Chromatography systems[3] or used in biopigment-based extraction-dyeing approaches for textiles.[4] Ultimately, this talk will showcase the transformative potential of ATPS in advancing the circularization of downstream processing and reveal key strategies for their commercial and successful implementation.

Keywords: Aqueous two-phase systems, Downstream processing, Circular bioprocesses, Liquid-liquid extraction, Bioproducts

Acknowledgments

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First-principles models in bio materials description: do we need them at all?

Matej Huš[1]

[1]Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, 1000 Ljubljana, Slovenia

Contemporary quantum chemical methods stem from physics and materials science, where they have been used rather routinely since 1980s. In the late 1990s and early 2000s, their use has been expanded first to individual small molecules and later to describing increasingly large molecules and chemical systems.

In the past, their accuracy of first principles simulations was insufficient for chemical purposes, but modern approaches have reached chemical precision. Nowadays, they are used to predict reactivity, reaction rates and product distributions. However, they are often still referred to as trend-describing methods rather than quantitatively accurate descriptions.

Recently, research has focused towards simultaneously describing reactions at different scales, which requires the use of different tools. In multiscale models, we need to introduce a flow of information between the different levels of simulations. These commonly include atomistic calculations, kinetic modelling and reactor level modelling. The exact structure depends on the goal of the simulations.

In general, we can use modelling either to understand the fundamentals of the process or to explain and predict the behaviour. In this contribution, we will present some examples where multiscale modelling based on first principles was used to explain the experimental observations (nitration of phenols), to understand the reaction mechanism (methane dry reforming), to explain hydrophobicity of differently treated nanocellulose, to describe the changes of the catalyst surface during the reaction (propane dehydrogenation), rapidly screen ligands in homogeneous catalysis (hydroarylation), and to screen the periodic system for better catalysts (ethylene epoxidation).

Lastly, we will address the question whether first-principles methods are useful for describing bio-based materials on account of their size.

Keywords: Ab initio modelling, Materials science, Catalysis

Acknowledgments

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In harmony with nature: unlocking the sustainable potential of glycine betaine in agrochemistry and surfactants

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To reduce the environmental impact of new chemicals, it is essential to derive substances from renewable sources and ensure they are easily biodegradable. Their synthesis should ideally employ non-toxic, reusable reaction media. Glycine betaine, a biodegradable and non-toxic compound, meets these criteria and can account for over 25% of the waste mass from sugar beet processing. By *O*-alkylating its carboxylate group, specific quaternary ammonium salts (QASs) with ester bonds can be synthesized. These esters hydrolyze rapidly into low-toxicity substances, reducing environmental pollution compared to fully synthetic QASs.[1,2]

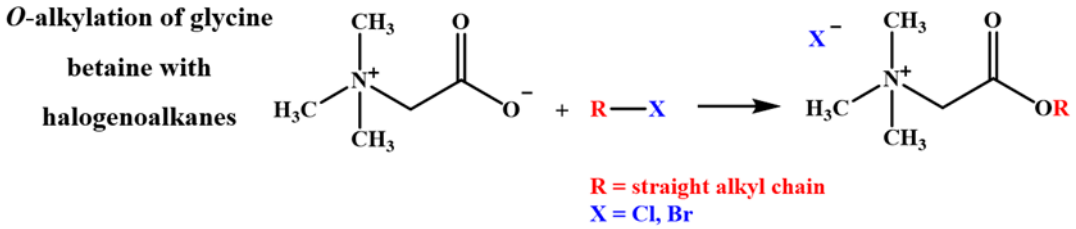

Figure 1. Synthesis of glycine betaine esters via O-alkylation reaction.

Currently available methods for synthesizing alkylated derivatives of glycine betaine require toxic reagents. Additionally, most are time-consuming and involve numerous unit operations. Therefore, efforts were made to improve the process and develop more favorable conditions for commercial-scale production. Optimization of betaine *O*-alkylation enables a shorter process, lowers synthesis costs, and reduces energy consumption. This research paves the way for scaling up betaine ester synthesis to large laboratory and industrial levels. Furthermore, promising results regarding their cleaning and herbicidal properties, along with ecotoxicity assessments, highlight their strong potential for commercial applications.

Keywords: Glycine betaine, Plant protection, Cleaning, Biological activity, Esters

Acknowledgments

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Oral presentations

High-Pressure Stirred Reactor System for Biomass Valorization

Maja Gabrič,[1,2] Žan Lavrič,[1,2] Brigita Hočevar,[1] Miha Grilc,[1,2] Blaž Likozar[1]

[1]Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, 1000 Ljubljana, Slovenia

[2] University of Nova Gorica, Vipavska Cesta 13, 5000 Nova Gorica, Slovenia

Biomass, comprising plant-derived materials such as lignocellulose, sugars, and waste oils, represents an abundant and renewable feedstock for the sustainable production of chemicals and materials. Efficient conversion of biomass into value-added products is a key strategy in the transition toward a circular, low-carbon economy. Our research group focuses on the complete valorization of biomass waste through catalytic, chemical, and enzymatic processes. To support this work, we utilize a modular high-pressure reactor system featuring six independently controlled, magnetically stirred 75 mL reactors (Figure 1). Each reactor can operate at temperatures up to 300 °C, pressures up to 200 bar, and stirring speeds up to 1000 rpm. The system features advanced temperature control mechanisms, including heating jackets, which ensure precise and consistent temperature control. The reactors are designed to operate under high pressure and can be pressurized with gases such as hydrogen (fume hood with sensors) or oxygen, with safety features ensuring safe operation under high pressure. The ability to run multiple reactions simultaneously increases throughput and reduces the time required for experimentation and optimization for biomass valorization and production of additional value c3 to c6 chemicals.

Figure1: Parr multi reactor system.

Keywords: Biomass utilization, Reaction engineering, Process optimization, Stirred reactor system

Acknowledgments

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Kinetic Modelling of Polyethylene Terephthalate Glycolysis

Žan Lavrič,[1] Maja Gabrič,[1] Miha Grilc[1]

[1] Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, SI 1000 Ljubljana, Slovenia

Polyethylene terephthalate (PET) is a versatile thermoplastic polymer that is widely used in the packaging industry, in the manufacturing of stretch bottles and in textile fibers.[1-2] This study presents a comprehensive investigation into the glycolysis of PET. The research encompassed the development of analytical methods, experimental work using various reactor systems, and the formulation of mathematical models to describe the process kinetics. Quantitative analysis of BHET was carried out using an optimized HPLC method, while a size-exclusion chromatography technique was established to determine the molecular weight distribution of the remaining solid PET. More than 33 experiments were conducted in magnetically coupled shaft-stirred Amar reactors, generating over 300 BHET concentration data points across a range of reaction times, temperatures, catalyst concentrations, and ethylene glycol to PET ratios. Based on these results, a kinetic model was developed and validated to capture the observed reaction behavior. The general predictions by kinetic model are shown in **Figure**.

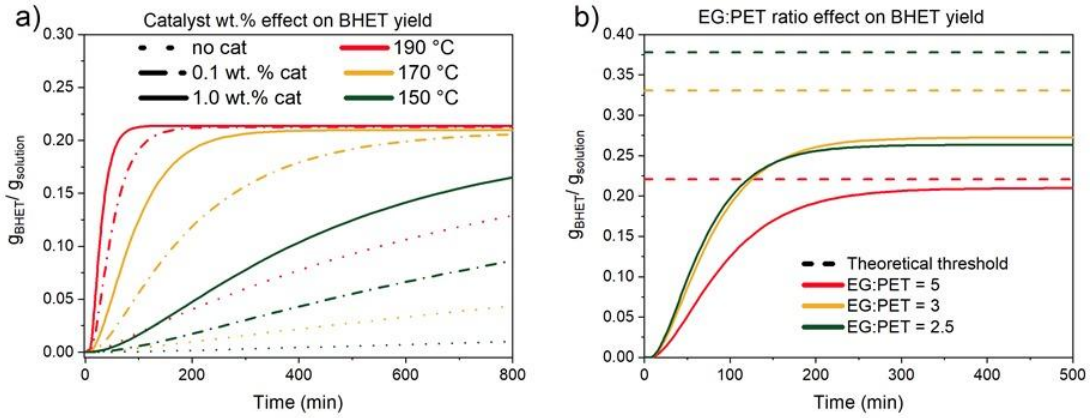

Figure 1: Kinetic model BHET yield prediction profiles. a) catalyst variation at three temperatures and EG to PET ratio of 5. b) EG to PET ratio variation and comparison with theoretical yield, at 170 °C, 1.0 wt.%.

Keywords: PET depolymerisation, Glycolysis, Homogeneous catalysis, Kinetic modelling

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Electrified methanation: using magnetic heating for efficient, on-demand in-situ fuel production

Anej Blažič,[1] Janvit Teržan,[1] Anja Sedminek,[2] Žan Kovačič,[1] David Bajec,[1] Sašo Gyergyek,[2] Blaž Likozar[1]

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Methanation is a catalyzed, exothermic reaction between carbon dioxide (CO_2) and hydrogen (H_2) in which methane (CH_4) and water (H_2O) are formed. The catalytic conversion of CO_2 provides a unique way to convert captured CO_2 into carbon-based fuels, storing excess renewable energy as chemical energy. This concept is the basis for the emerging Power-to-X (P2X) technology, where green H_2 is used for the on-demand in-situ production of carbon-neutral synthetic fuels such as CH_4, methanol and ammonia. [1]

In this study, the methanation reaction was carried out using a magnetic heating, which enables a rapid temperature rise, precise temperature control and uniform heating of the catalyst. The methanation reaction was studied with a magnetic cobalt-nickel-alumina nanocomposite ($Co_{0.7}Ni_{0.3}$-Al_2O_3) prepared according to the synthesis described in study. [2] Three different nanocomposites were tested: two with different aluminum oxide content (CN-A50, CN-A70) and a third with ruthenium nanoparticles precipitated on the surface of nanocomposite (CN-A50-1Ru).

The highest CO_2 conversions were achieved with the CN-A50-1Ru catalyst due to its superior ability to activate hydrogen, which in turn lowers the activation energy for CO_2 hydrogenation. [3] In addition, the catalytic activity of the catalysts directly correlated with the number of active sites determined by CO pulse adsorption measurements, reflecting the amount of accessible metal. DFT calculations revealed that the most thermodynamically favorable pathway is the hydrogenation of CO_2 to form a COOH* intermediate, which dissociates into CO*. The latter is then further dissociated to C*, which is subsequently hydrogenated to CH_4.

Keywords: Magnetic heating, Power-to-X (P2X) technology, Methanation, CO_2 valorization

Acknowledgments

I would also like to express my gratitude to the European Space Agency (ESA) for providing the necessary resources.

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Application of chitosan-admixed hydrogels as electrode coatings

Vojtěch Škopek,[1,2] Filipa A. Vicente,[1] Blaž Likozar,[1] Ilja Gasan Osojnik Črnivec[1]

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[2] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, Ljubljana SI-1000, Slovenia

This research focuses on the development of bio-based hydrogels derived from chitosan, alone or in combination with other polysaccharide matrices, as functional coatings for metal electrodes in water electrolysis. The main objective is to explore the potential of covalently crosslinked aerophobic hydrogels to enhance the hydrogen evolution reaction by facilitating gas bubble detachment from electrode surfaces. This approach aims to reduce overpotentials and improve the kinetics of hydrogen production, ultimately increasing the overall efficiency of the electrolysis process.

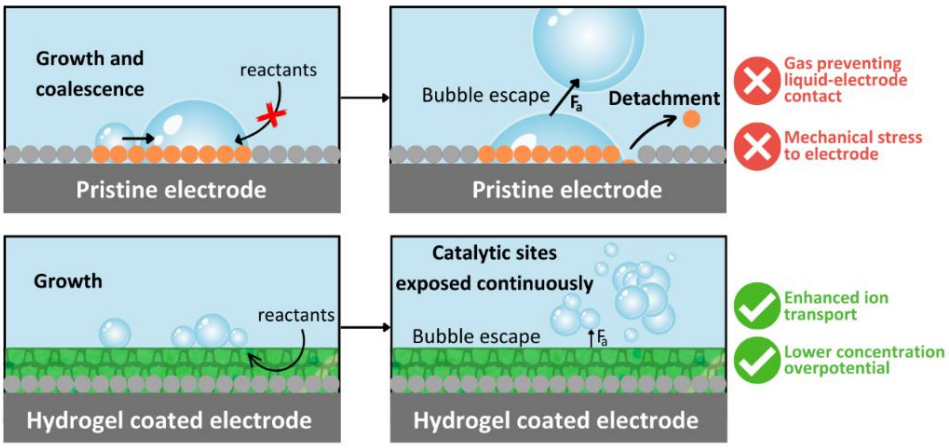

Figure 1: Graphical comparison between a pristine electrode and a coated electrode

Aligned with the goals of green chemistry and circular economy, this work contributes to the development of innovative and environmentally friendly technologies that support sustainable industrial practices. Preliminary results demonstrate that the synthesized bio-based hydrogels exhibit good mechanical and chemical stability, as confirmed by gelation tests, while maintaining aerophobic characteristics suitable for electrochemical applications.

The effect of different coating techniques, such as spin-coating and dip-coating, will be investigated to optimize hydrogel adhesion and thickness on metal substrates, including platinum and nickel electrodes. Electrochemical performance will be evaluated in a half-cell setup using reversible hydrogen reference electrode and KOH electrolyte across a range of alkaline pH values. Preliminary results suggest that these bio-based hydrogel coatings can significantly enhance hydrogen production efficiency, offering a sustainable and high-performance alternative to conventional synthetic polymer coatings used in water electrolysis.

Keywords: Coating, Hydrogel, Electrolysis, Hydrogen

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Design, Engineering, and Applications of Enzymes for Sustainable Biocatalytic Processes

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Enzyme-based catalysis offers a sustainable alternative to conventional chemical processes, aligning with the principles of the circular economy. Advances in the design and application of free and immobilized enzymes for enhanced stability, reusability, and catalytic performance in environmentally relevant processes. Enzymes can be immobilized on low-cost lignocellulosic supports (e.g., green coconut fibers and bacterial cellulose) and on nanomaterials (e.g. carbon xerogels and carbon nanotubes), achieving high activity retention and improved operational stability for the polymerization of diverse compounds, degradation of various pollutants in aqueous media[1–4]. On the other hand, aqueous biphasic systems were developed as liquid-phase supports for enzyme immobilization (e.g. composed of cholinium-based ionic liquids and polymers), enabling complete enzymatic reactions with high enzyme recovery and recyclability over multiple cycles[5,6]. These works demonstrate that combining material engineering with biocatalyst optimization enables robust, efficient, and recyclable enzyme systems suitable for industrial bioprocesses and environmental bioremediation (Figure 1). Its broader application will be further stimulated in the future by the emerging biobased economy.

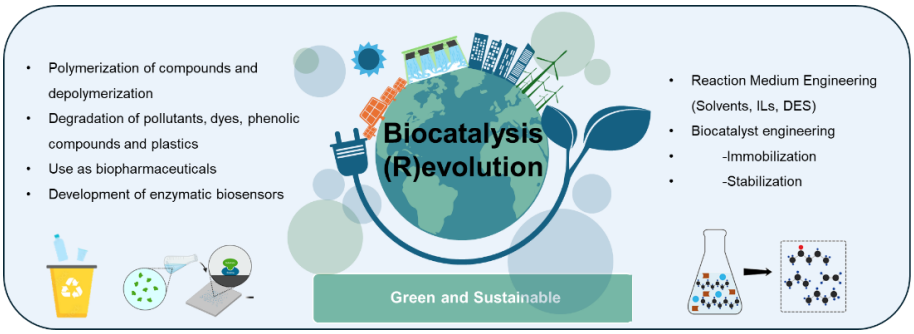

Figure 1: Biocatalysis for sustainable enzyme applications.

Keywords: Enzymes; Biocatalysis; Immobilization; Reuse ; Applications

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From plant to paper: sustainable curcuminoid extraction for paper-based applications

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The current global crisis is marked by a concerning buildup of waste and no action being taken, posing a serious threat to environmental sustainability. This urgent situation underlines the necessity for immediate adoption of sustainable practices and the development of innovative solutions to confront increasing ecological issues and safeguard our planet's future. In light of these challenges, the present study introduces an environmentally friendly method for extracting curcuminoids from *Curcuma longa* using micellar solutions. This approach contributes to lowering the environmental impact of extraction technologies by combining two stages: solid–liquid extraction (SLE) and liquid–liquid extraction (LLE), into a more efficient process. The SLE step employs a buffer solution mixed with a biodegradable surfactant, leading to the formation of an aqueous micellar two-phase system (AMTPS), a specific subtype of LLE. This integration not only simplifies the procedure but also adheres to green chemistry principles by reducing the use of harmful solvents. Optimization of the SLE and LLE conditions enabled the recovery of more than 95% of curcuminoids into the surfactant-rich phase. Furthermore, the resulting surfactant-rich extract exhibited notable stability, maintaining its integrity after more than 50 hours of UV exposure with only around 20% degradation, compared to approximately 40% degradation in the control sample. Additional tests confirmed the system's thermal stability, reinforcing its suitability for applications where curcuminoids are exposed to light and heat. These systems were incorporated into papermaking to test color fading under various conditions, including paper ageing.

Keywords: Curcuminoids, Aqueous micellar two-phase systems (AMTPS), Biodegradable surfactant

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Innovative processes for protein extraction and recovery from insects

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The growing global population is expected to increase the demand for meat-based protein, raising concerns regarding sustainability, environmental degradation, and resource inefficiency. Therefore, it is essential to identify alternative protein sources, with insects standing out as a highly promising option for sustainable food systems. Conventional methods for insect protein extraction typically rely on aqueous alkaline solutions, followed by lengthy and costly downstream processing steps. These approaches often result in limited protein yields and the formation of undesirable protein–phenolic complexes.

In this work, we developed different strategies for the extraction and purification/recovery of proteins from edible insect flours (*Tenebrio molitor*, *Acheta domesticus* and *Hermetia illucens*), aiming their application in innovative food products. A systematic study of greener solvents – comprising non-toxic conventional solvents and alternative solvents – was conducted to establish different efficient protein extraction processes. Solvents were prepared and characterized, and then applied for the extraction. The processes were optimized in terms of operation conditions (*e.g.* solvent concentration, time, temperature, liquid-solid ratio, *etc*) to maximize the protein yield. The scalability of the processes was also studied. Therefore, several innovative approaches were successfully developed for the extraction and valorization of proteins from insects, representing a stepping-stone towards the use of insect-derives products in human food.

Keywords: Insects, Proteins, Extraction, Recovery, Alternative Solvents.

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Eco-Friendly Extraction of Insect Oils from the Portuguese Bioindustry

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The continuous growth of the global human population and the decline of investment in agriculture, forestry and fishing pose a problem of nutrient shortage. The Food and Agriculture Organization of the United Nations (FAO) points that "the world is still far off track to achieve Sustainable Development Goal (SDG) 2, Zero Hunger, with the global prevalence of undernourishment persisting at nearly the same level for three consecutive years after having risen sharply in the wake of the COVID-19 pandemic".[1] Thus, edible insects can become a valuable alternative for animal-derived protein [2] and oil [3]. Indeed, insect farming can help overcome the hunger problem, with this research area currently expanding rapidly. There are already several companies in Portugal dedicated to insect farming.[4] Through a partnership project with these companies, insect flours and insect larvae were obtained to search for sustainable oil and protein extraction processes (Figure 1a).[5] In this work, the optimization of oil extraction from insect flours, such as: (i) *Tenebrio molitor* (mealworm) larvae, (ii) *Acheta domesticus* (domestic cricket), and (iii) *Hermetia illucens* (black soldier fly), was attained by sustainable technology. Solid-liquid extraction procedures were developed using green solvents at room temperature. The oils from *Tenebrio molitor* and *Hermetia illucens* were essentially composed of triacylglycerols (TAG, Figure 1b), while the oil from Acheta domesticus was primarily made of free fatty acids. The extracts were characterized by classical techniques including including NMR and MS/MS.

(a) 

(b) 

Figure 1: (a) InsectERA partnership; (b) TAG generic structure.

Keywords: Edible insects, Oil extraction, Green solvents, Insect farming, Food sustainability

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Accelerating Sustainable Materials Discovery with Artificial Intelligence

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The development of sustainable materials, particularly green solvents, is a critical challenge in the transition towards a circular economy. Many promising solutions, such as deep eutectic solvents (DESs), are complex, multicomponent mixtures whose properties are tunable through careful selection of molecular precursors and compositions. However, discovering optimal formulations through traditional trial-and-error experimentation remains costly, labor-intensive, and time-consuming.

In this work, artificial intelligence (AI), particularly stochastic machine learning models like Gaussian processes (GPs), are leveraged to significantly accelerate the discovery and optimization of sustainable materials. GPs excel in low-data regimes, efficiently interpolating sparse experimental datasets while quantifying uncertainty. This makes them ideal for guiding iterative experimentation via active learning or Bayesian optimization, effectively turning GPs into laboratory companions.

Through several case studies, this work demonstrates how GPs can reduce the experimental burden in solvent design, including the construction of phase diagrams, prediction of solubility curves, and estimation of physicochemical properties from quantum chemistry descriptors (*e.g.*, sigma profiles). Beyond predictive accuracy, the interpretability of GP models provides valuable insights into structure–property relationships, effectively allowing models to "learn chemistry" from limited data. These capabilities position stochastic AI approaches as powerful laboratory companions in the search for sustainable materials, helping accelerate innovation while minimizing environmental and experimental costs.

Keywords: Gaussian processes, Machine learning, Green chemistry, Bayesian optimization

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Permeation Modeling of Porous Membrane in a Direct Contact Membrane Distillation Module

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Membrane distillation (MD) is a separation process commonly used in water treatment (*e.g.* solution concentration). This separation process utilizes a hydrophobic membrane to separate the permeate and feed side of the module. The distillation process is driven by the vapor pressure difference on hot feed side and cold permeate side of the hydrophobic membrane. MD utilizes low grade heat to evaporate volatile compounds, usually at temperatures lower than boiling point. Due to low flux, process optimization is necessary for industrial implementation. Modeling such processes with Computational Fluid Dynamics (CFD) can aid in process development, module design and helps eliminating the need for unnecessary experimental setups and reducing research cost [1–4].

Modeling of membrane permeation was approached by theoretical diffusion model using a combination of diffusion models, theoretical membrane characteristic models and CFD simulation of a direct membrane distillation model. Effects of temperature polarization were considered. Membrane surface was 30 cm^2, membrane porosity was 0.75, thickness was 125 μm and water contact angle was 130.2°. Extracted data from the simulation was used to calculate the total flux using Dusty Gas model and Maxwell derived diffusion equation. The model results were compared to experimental data from literature. The aim was to study mass transfer flux and polarization effects to find the best fit parameters to experimental data.

Keywords: Membrane distillation, Permeation modeling, Computational fluid dynamics

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CFD in Real-World Engineering

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Despite major technological advances, the reaction mechanisms and surface properties of catalytic systems are still not fully understood. Understanding how reactants interact with catalytic surfaces remains a central focus of academic research. Multi-scale hierarchical modelling—covering atomistic to macro scales—has shown success in simulating complex industrial processes involving heterogeneous catalysis. However, this approach demands significant computational resources, limiting its use in industrial settings.

A more practical alternative is Computational Fluid Dynamics (CFD), which is widely used in chemical engineering for simulating fluid flow, heat and mass transfer, and chemical reactions. CFD provides detailed insights into local conditions such as temperature, pressure, velocity, concentration, and reaction rates. This helps optimize the design of reactors, mixers, heat exchangers, and other chemical equipment.

One challenge in applying CFD in industry is linking its detailed results to simplified continuum models used in engineering practice. These models assume homogeneous fluid properties and rely on empirical correlation equations (CEs)—such as those for heat and mass transfer—based on dimensionless numbers (Reynolds, Nusselt, Sherwood, *etc.*). While useful for quick calculations in models like plug flow or stirred tank reactors, CEs have limitations. They require system-specific experimental calibration, apply only within limited operating ranges, and fail to capture local fluid dynamics.

To address these issues, a new method uses CFD to derive effective CEs by averaging local dimensionless quantities across the domain. This embeds complex phenomena like turbulence, geometry, and kinetics into simplified models, improving accuracy and reducing the need for experiments.

This approach enables rapid, reliable process optimization and extends CE applicability, benefiting systems such as gas-liquid reactors, spray dryers, and nanofluid heat exchangers—striking a balance between precision and computational efficiency.

Keywords: Correlation equations, Mass and heat transfer, Model order reduction, CFD

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Reshaping Sample Pretreatment for Clinical Bioanalysis

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Clinical biomarkers are central to modern medicine, contributing to improved patient care. Despite their critical importance, clinical bioanalysis continues to face challenges in accurately quantifying biomarkers in complex human samples. High-abundance endogenous components frequently interfere with the detection of low-abundance targets, making sample pretreatment an indispensable step in bioanalytical workflows. Conventional methods, however, often suffer from limited selectivity and low biomarker recovery, while relying on resource-intensive protocols.[1]

To overcome these limitations, alternative strategies that combine high analytical performance with sustainability are urgently required. In this context, ionic liquids (ILs) have emerged as versatile tools, offering tunable physicochemical properties and selective interactions with biological matrices.[2] This presentation showcases our recent developments in IL-based sample pretreatment technologies, exploring their dual role in two complementary formats: as phase-forming agents in LLE via aqueous biphasic systems and as functionalized supports in SPE. Successfully applied to various samples, including blood, urine, and saliva, these approaches reduce matrix effects and improve biomarker recovery.

In addition, this presentation features recent advances by our group in the integration of these IL-based pretreatment technologies into point-of-care (PoC) devices. In particular, the combination of IL-based aqueous biphasic systems with microfluidic platforms has shown enhanced sensitivity compared to untreated samples.[3]

By reshaping sample pretreatment within the context of clinical bioanalysis, this work advances the development of more effective, sustainable, and accessible diagnostic platforms.

Keywords: Ionic liquids; Sample pretreatment; Aqueous biphasic systems; Point-of-care devices; Clinical biomarker

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Manufacturing, preservation, and delivery of biopharmaceuticals@PATh

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Biopharmaceuticals, including proteins and nucleic acids, have become essential medicines in healthcare systems for the prophylaxis and treatment of chronic and life-threatening diseases. However, their manufacturing involves complex upstream and downstream processes, which considerably impact their cost. Adding to this challenge are the bioavailability and pharmacokinetics of common biotherapeutics, leading to unmet clinical demands, safety concerns, and poor patient compliance. With the aim of developing efficient biological materials to tackle health priority diseases, our team has been exploring the use of neoteric solvents (ionic liquids – ILs, and deep eutectic solvents – DES) and related materials, viz., supported ionic liquids and ionogels. These innovative systems are being applied to advance both downstream processing and formulation (including stabilization and delivery) of biopharmaceuticals, particularly therapeutic proteins and nucleic acids (*e.g.*, plasmid DNA and messenger RNA).[1] This presentation provides an overview of the technologies currently in use in our labs to produce biopharmaceuticals, which leverage recombinant bacteria/yeast, and enzymatic processes. It then highlights key studies demonstrating the successful application of aqueous biphasic systems and IL-functionalized chromatographic supports for the clarification and purification of these products. The final section focuses on ongoing research efforts aimed at improving the stability and delivery of biotherapeutics using non-invasive routes of administration. Overall, our findings suggest that ILs/DES-related technologies hold significant promise in creating efficient and more sustainable methods for the manufacturing and formulation of biopharmaceuticals.

Keywords: Biopharmaceutical; Purification; Formulation; Ionic liquid; Deep Eutectic Solvent.

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Strategies for the exploitation of natural compounds: from extraction to valuable applications

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Among the variety of promising high-value compounds that can be obtained from natural resources, lipophilic, such as sterols, terpenes and fatty acids, and phenolic compounds have attracted attention due to their health-promoting properties, including anti-inflammatory, antibacterial or antiproliferative activities,[1-2] making them very promising for nutraceutical, cosmetic or pharmaceutical applications. However, a major challenge remains: the development of environmentally friendly and efficient extraction methodologies.

Different methodologies have been explored in order to recover these bioactive compounds from natural resources, namely, supercritical fluid extraction (SFE),[3] high-pressure assisted extraction (HPE),[4] microwave-assisted extraction (MAE) and more recently extraction with alternative solvents, namely switchable, bio-based and eutectic solvents.[5] Some of these solvents have become particularly interesting, as they can be used as formulation media and to enhance biological activities. In this talk different case studies using the above mentioned methodologies will be presented, involving both lipophilic and phenolic compounds obtained from different natural resources. The rationale behind the selection between different methodologies, how some techniques can be more selective than others, how predictive models can be used to select alternative solvents and how bioactivities can be improved will be afforded. It is intended to show which strategies can pave the way for the exploitation of natural compounds in high-value applications.

Keywords: Bioactive compounds, Natural resources, Sustainable extraction, High-value applications.

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Solvent design for hydrometallurgy – application to lithium-ion battery recycling

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The increasing electrification of modern society is heavily dependent on electronic and energy storage devices, with lithium-ion batteries (LIBs) playing a pivotal role. Since their introduction to the market, their features — such as high energy density, large capacity, long cycle life, and minimal maintenance requirements — made them indispensable to the energy industry. As a result, the demand for LIBs is expected to grow by over twenty percent yearly by 2030,[1] stimulating demand for critical metals like lithium, cobalt, nickel, and manganese. End-of-life (EoL) LIBs present a valuable opportunity as a source of these metals, often offering higher concentrations compared to traditional mineral ores,[2] whilst their adequate management minimises environmental pollution, resource losses, and supply chain risks.[3] Although battery repurposing will also play a relevant role, the recycling industry will continue growing in the coming years driven by recent EU legislation (Regulation (EU) 2023/1542), with batteries from 2031 onwards requiring a minimum recycled content of 6 % Li, 16 % Co and 6 % Ni and further increased by 2036.

This presentation showcases the recent work at the DESignSX research group exploring the transition of EoL LIBs down the waste hierarchy, exemplifying reuse strategies for the cathodic black mass before advancing to hydrometallurgical recycling with a focus on exploiting non-aqueous solvents for the design of alternative recovery processes.

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Ionic and Eutectic Systems as versatile (bio)materials for energy, water purification and therapeutic applications

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Ionic and eutectic systems represent a highly versatile class of materials, offering tunable physicochemical properties that support a broad spectrum of applications in energy, environmental remediation, and biomedicine. Their structural flexibility, low volatility, and functional adaptability make them ideal candidates for next-generation sustainable technologies. In the field of **energy**, Ionic Liquids (ILs) and eutectics facilitate key processes such as CO_2 valorization to fuels or acting as efficient electrolytes for energy storage devices. Their ability to stabilize metal nanoparticles enables efficient CO_2 methanation at moderate temperatures, achieving high methane yields.[1] Complementary approaches using ILs or eutectic-based electrolytes are promissory materials for application in batteries, dye-sensitized solar cells (DSSCs) and supercapacitors.[2] For **water purification**, hydrophobic eutectics and ionic covalent organic frameworks (iCOFs) offer an efficient platform for extracting and removing organic pollutants and heavy metals from contaminated water sources.[3] Their selectivity, reusability, and low environmental impact present a sustainable alternative to conventional solvents. In **therapeutics**, ILs have demonstrated significant potential as bioactive solvents and delivery agents. By pairing ionizable active pharmaceutical ingredients (APIs) with biocompatible counter-ions, enhance the original solubility, stability, and bioavailability of drugs. Our group has developed pharmaceutical ILs and organic salts based on antimicrobial, anticancer and antiviral agents, showing superior therapeutic performance.[4] When integrated into silica nanoparticles, these systems exhibit enhanced antibacterial activity, offering a promising strategy to overcome drug resistance and enable targeted drug delivery. Together, ionic and eutectic systems offer a unique convergence of functionality and sustainability, positioning them as promising materials for the future applications.

Keywords: Ionic (bio)materials, Eutectic systems, Sustainable energy, Water purification, Therapeutics

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