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Perspectives in Analytical & Physical Chemistry (APC)

APC - D4 - P01
A polymer-based surface functionalization strategy for DNA immobilization on gold electrodes

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Surface functionalization is a critical step in the development of electrochemical DNA biosensors. Gold electrodes are widely used due to the well-established Au–SH chemistry, which enables the immobilization of thiolated DNA probes. However, thiol-based strategies often require time-consuming probe activation and suffer from limited long-term stability, as the Au–S bond is weaker than covalent linkages and prone to desorption and oxidation processes [1]. Here, we present a polymer-based coating strategy to rapidly and simply functionalize gold electrodes for DNA probe immobilization. The polymer was successfully applied to gold surfaces, The polymer was successfully applied to gold surfaces, as confirmed by electrochemical impedance spectroscopy. As shown in Figure 1, a marked increase in charge transfer resistance (Rct) was observed after polymer coating and subsequent DNA probe immobilization, indicating effective surface functionalization. Importantly, the polymer coating did not significantly alter the double-layer capacitance of the electrode, while providing antifouling properties. Overall, this approach enables a simple and robust functionalization of gold electrodes via hydrophobic interactions, offering a versatile platform for DNA-based electrochemical biosensing.

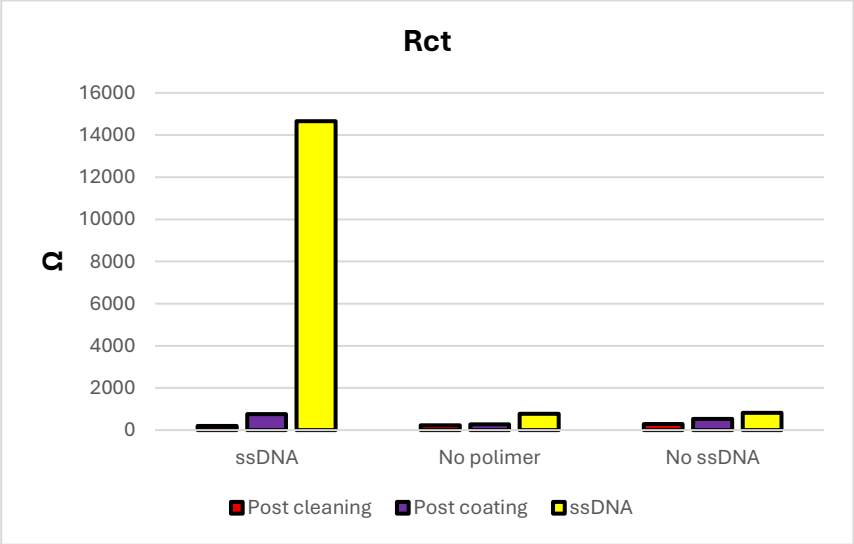

Fig. 1. Comparison of the charge transfer resistance (Rct) after surface functionalization.

[1]Love, J. C.; Estroff, L. A.; Kriebel, J. K.; Nuzzo, R. G.; Whitesides, G. M. Self-Assembled Monolayers of Thiolates on Metals as a Form of Nanotechnology. Chem. Rev. 2005, 105, 1103–1169.

APC - D4 - P05
Exciton spatiotemporal imaging: From classical diffusion to quantum correlations

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Carrier dynamics are a key determinant of semiconductor device performance. However, studying carrier dynamics in nanometer/femtosecond scales under multi-physical field conditions is highly challenging. To overcome this bottleneck, we developed a wide-field transient optical microscope compatible with multiple physical fields. It achieves 300 fs time resolution, 30 nm spatial accuracy, and 10^{-5} OD sensitivity under 4 K, electric field, and 1 fps frame rate conditions. With this technology, we first realized optical imaging of the ultrafast transport process of excitons in two-dimensional perovskite materials[1], measuring their exciton diffusion rate and exciton annihilation coefficient. Further, we extended our field of view to the Moiré superlattice of two-dimensional transition metal dichalcogenides with strong correlation effects[2]. In this material, carrier behavior is no longer merely a classical diffusion process but is significantly influenced by quantum correlation effects. The strong long-range dipole repulsion between excitons leads to a "freezing" phenomenon in the dynamic behavior of the exciton Mott insulator, lasting up to 70 nanoseconds. This challenges the classical theory of repulsive forces dispersing particles and highlights the unique properties of quantum transport. These findings not only expand our understanding of exciton dynamics in low-dimensional materials but also provide new insights and theoretical foundations for the development of quantum information technologies and efficient optoelectronic devices.

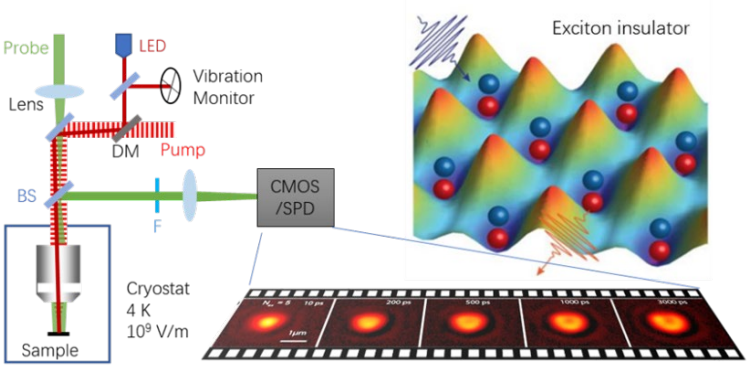

Fig. 1. Transient optical imaging of exciton dynamics.

Keywords: Transient absorption microscopy, transient fluorescence, exciton dynamics, Van der Waals heterostructures, interface interactions

[1]S. Deng, E. Shi, L. Yuan, L. Jin, L. Dou, L. Huang, *Nature Communications*, 11 (**2020**) 664.
[2]S. Deng, H. Park, J. Reimann, J.M. Peterson, D.D. Blach, M.-J. Sun, T. Yan, D. Sun, T. Taniguchi, K. Watanabe, X. Xu, D.M. Kennes, L. Huang, *Nature Materials*, 24 (**2025**) 527-534.

APC - D4 - P06

Untargeted UHPLC–IMS–M metabolomics reveals genotype-dependent chemical diversity among avocado varieties

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The global avocado market is largely dominated by the Hass variety due to its desirable sensory attributes, resistance to transport, extended postharvest shelf life, and the ease of monitoring ripening through characteristic skin colour changes. However, numerous less-studied avocado varieties exist and may represent promising alternatives in terms of agronomic performance, nutritional value, and opportunities for product diversification. A comprehensive understanding of the compositional differences among these varieties is essential before considering their potential introduction into commercial markets. In this context, metabolomic approaches provide powerful tools for the comprehensive characterization of fruit composition and for exploring metabolic variability associated with genetic background.

This study investigated the metabolomic profiles of 31 avocado varieties using an untargeted approach based on UHPLC–IMS–MS/MS. The varieties were classified into three groups according to their genetic background: *Hass* mutations, *Hass* descendants, and non-related varieties. Methanolic extracts obtained from freeze-dried mesocarp samples were analyzed using a UHPLC–timsTOF platform. The incorporation of collision cross section (CCS) values provided an additional molecular descriptor, enhancing annotation confidence through comparison with in-house spectral libraries, public databases, and in silico–predicted CCS values.

More than 100 metabolites were tentatively identified across all samples, including sugars, organic acids, amino acids, nucleosides, vitamins, and phenolic compounds (e.g., phenolic acids and flavonoids), as well as other metabolites relevant to fruit quality and nutritional value. Multivariate statistical analysis revealed distinct clustering patterns associated with genetic origin. Non-related varieties were widely dispersed across the PCA scores plot, indicating a high degree of metabolic diversity. In contrast, Hass mutations and Hass descendants formed compact, well-defined clusters clearly separated from the remaining varieties. Supervised PLS-DA models showed good fit and predictive performance, enabling the identification of discriminant metabolites responsible for class separation and suggesting their potential as genetic markers.

APC - D4 - P07

Postharvest storage and on-tree maturation drive distinct carbohydrate signatures in *hass* avocado

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Avocado (*Persea americana* Mill.) is widely appreciated for its culinary and nutritional value. However, meeting the increasing global demand often relies on imported fruit that undergoes prolonged cold storage during transport. As a climacteric fruit, avocado ripens after harvest, and non-structural carbohydrates play a central role in this process. Despite their importance, the biochemical mechanisms governing carbohydrate dynamics during ripening and postharvest handling remain only partially understood.

This study evaluated how postharvest management influences the carbohydrate profile of *Hass* avocado mesocarp at edible ripeness by comparing prolonged cold storage with extended on-tree maturation. Approximately 125 fruits were harvested and stored under controlled temperature and humidity conditions in refrigerated chambers to simulate typical transport logistics. At 10-day intervals, subsets of fruits were removed from cold storage and allowed to ripen at room temperature until reaching edible ripeness. In parallel, freshly harvested avocados were collected from the trees at each time point and ripened under the same conditions to represent domestic supply scenarios. Five biological replicates, each consisting of five fruits, were analyzed per time point. Freeze-dried mesocarp samples were extracted using ultrasound-assisted solid–liquid extraction with a 60:40 (v/v) ethanol–water mixture, and the resulting extracts were analyzed by hydrophilic interaction liquid chromatography coupled with mass spectrometry (HILIC–MS).

The results revealed that cold-stored avocados exhibited a progressive accumulation of seven-carbon (C7) sugars, particularly perseitol and *D*-mannoheptulose. In contrast, fruits that remained longer on the tree accumulated higher levels of six-carbon (C6) sugars, including glucose, fructose, and sucrose. Principal component analysis (PCA) confirmed a clear separation between cold-stored and freshly harvested samples, highlighting the strong influence of postharvest conditions on avocado carbohydrate metabolism.

These findings provide new insights into how harvest timing and storage practices shape avocado metabolic composition, offering valuable guidance for improving postharvest management, optimizing supply chains, and enhancing fruit quality.

APC - D4 - P08
Surfactant-free microemulsions in surface cleaning

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Classical microemulsions are transparent, thermodynamically stable liquid systems composed of two immiscible phases, stabilized by amphiphilic molecules commonly referred to as surfactants. These molecules accumulate at the oil–water interface, lowering the interfacial tension and enabling the formation of oil-in-water, bicontinuous or water-in-oil structures.[1]
Beyond conventional systems, nanostructured single-phase solutions can be obtained without surfactants by incorporating hydrotropes. Unlike surfactants, hydrotropes are relatively small molecules with limited amphiphilic properties. Consequently, they neither form micelles in an aqueous solution nor create ordered interfacial films at the oil–water interface.[2,3] In ternary mixtures, these conditions can lead to the formation of surfactant-free microemulsions (SFMEs), which occur within the monophasic region above the phase boundary. The composition of these systems affects the observed structural regimes, with oil-in-water-like organizations typically associated with the so-called pre-Ouzo region.[4]
The nanostructuring in SFMEs is characterized by highly dynamic behavior and comparatively weak interfacial stabilization. Consequently, these systems exhibit pronounced mesoscale fluctuations and a high degree of structural flexibility. This combination of characteristics makes SFMEs a promising, environmentally friendly alternative for a variety of applications. In the context of surface cleaning, a detailed understanding of their dynamic structuring is essential to clarify their influence on cleaning efficiency and the underlying mechanisms.

[1]Kumar P., Mittal KL; Handbook of microemulsion science and technology. *New York: Marcel Dekker*; **1999**.
[2]Kunz W., Holmberg K., Zemb T.; *Curr Opin Colloid Interface Sci* **2016**, *22*, 99–107.
[3]Hou W., Xu J.; *Curr Opin Colloid Interface Sci* **2016**, *25*, 67–74.
[4]Klossek M. L., Touraud D., Zemb T., Kunz W.; *ChemPhysChem* **2012**, *18*, 4116-4119.

APC - D4 - P09
Characterization of tristyrylphenol ethoxylate surfactants

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Surfactants comprise a broad class of amphiphilic compounds with applications like household products or industrial processes. A large proportion of their overall consumption occurs in industry, where their performance must be precisely tailored through structural design to meet specific functional requirements.[1]
Tristyrylphenol ethoxylates are nonionic surfactants distinguished by an extended aromatic core and a variable ethylene oxide chain length. While they are mainly employed in agrochemical formulations[2], their structural characteristics also indicate potential in fields such as pigment and dye processing[3], petrochemistry, and materials science. The pronounced aromatic moiety enables interactions with π-conjugated systems of other aromatic compounds, which may enhance the solubilization of such poorly water-soluble molecules. In particular, these surfactants can disrupt intermolecular π–π stacking, allowing subsequent solubilization via their hydrophilic segments.
However, these surfactants remain insufficiently characterized in the literature. Therefore, their fundamental physicochemical properties and solubilization mechanisms are systematically investigated using techniques such as UV–Vis spectroscopy, NMR and DLS measurements, complemented by measurements of surface tension, foaming behavior, rheology, and phase behavior in binary and ternary systems containing hydrophobic and aromatic solutes.

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[1]Karsa D. R., Houston J., What are Surfactants?. Chemistry and Technology of Surfactants; Farn R. J.; Wiley, 2006; pp 1-21.
[2]Grubelmann-Bonneau, I. V. et al., Tristyrylphenol Surfactants in Agricultural Formulations : Properties and Challenges in Applications. Pesticide Formulations and Application Systems ; Hall F.R. et al.; ASTM, 1995; pp 119-136.
[3]Dário, B. S. et al. Tristyrylphenol based surfactants as efficient dispersants of TiO2 particles in dilute and concentrated dispersions. Colloids Surf. A Physicochem. Eng. Asp. 2022, 654, 130170.

APC - D4 - P10

Development and optimization of lipid nanocarrier systems for agri-food biowaste

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This study focuses on the circular bioeconomy, aiming to valorize agricultural by-products through the extraction and encapsulation of bioactive compounds for applications in the biocosmetic field. The research develops and optimizes lipid-based nanocarrier systems, specifically liposomes and solid lipid nanoparticles, designed to enhance physicochemical stability of labile molecules, improve bioavailability, and enable controlled release[1]. Nanocarriers are produced using environmentally sustainable approaches, based on biocompatible lipids and low-toxicity surfactants, in line with green formulation principles. Comprehensive physicochemical characterization is performed using advanced analytical techniques, including Dynamic Light Scattering[2] and Nuclear Magnetic Resonance[3]. Additional investigations include complementary techniques such as Scanning and Transmission Electron Microscopy, Fourier Transform Infrared Spectroscopy, and Small Angle X-Ray Scattering. A Quality by Design strategy, supported by Design of Experiments, is applied to optimize formulation variables and ensure robustness and reproducibility. Stability of the developed lipid nanocarriers is evaluated in complex dispersing media to support sustainable cosmetic formulations while preserving functional properties of encapsulated bioactives over time. The study also investigates the influence of formulation parameters on particle size, polydispersity, surface charge, and encapsulation efficiency, which are critical for stability and performance. Particular attention is given to the selection of raw materials derived from renewable sources, ensuring alignment with circular economy principles and reduction of environmental impact. Process conditions are carefully controlled to minimize energy consumption and solvent use, reinforcing sustainability goals. The resulting nanocarriers are further assessed for their potential incorporation into cosmetic matrices, evaluating compatibility, texture, and overall product stability. This integrated approach aims to provide scalable and reproducible solutions for the cosmetic industry, promoting innovation through the use of natural resources and advanced nanotechnology. Ultimately, the research contributes to the development of high-value products from agro-industrial residues, supporting sustainability and resource efficiency in modern formulation science while addressing consumer demand for safe, effective, eco-friendly products.

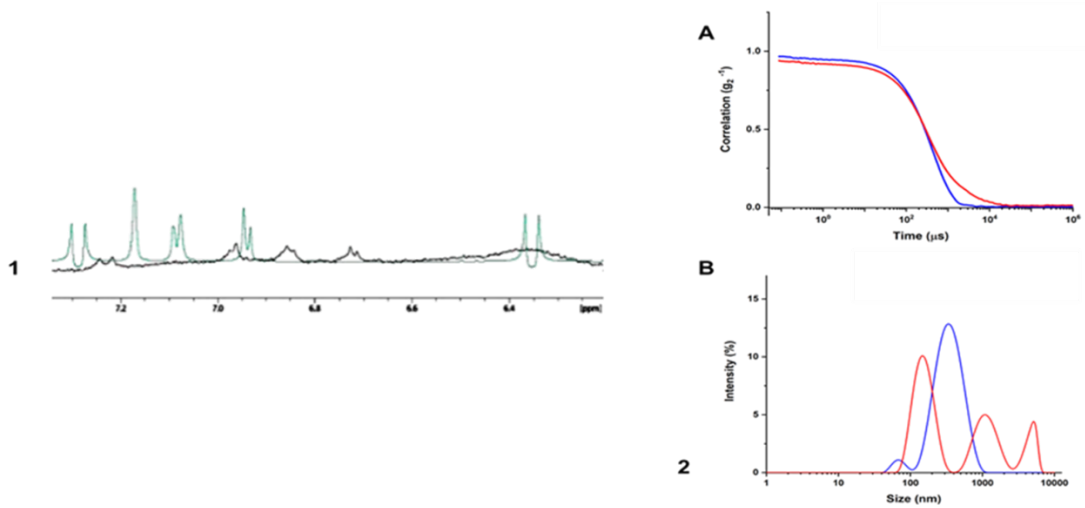

Fig. 1 [1]H NMR overlapped spectra of Caffeic Acid standard and Caffeic Acid encapsulated into DOPC-DOPE liposomes, in green and black, respectively
Fig. 2 Comparison of one-month stability between Sinapic Acid-loaded DOPC-DOPE liposomes and empty liposomes, in blue and red, respectively; Fig(2A): DLS Correlogram, Fig(2B): Intensity-based Size Distribution

[1]Katopodi, A.; Detsi, A. *Colloids and Surfaces A: Physiochemical and Engineering Aspetcs*. **2021**, 0927-7757
[2]Talarico, L.; Consumi, M.; Leone, G.; Tamasi, G.; Magnani, A. *Molecules* **2021**, *26, 2694*
[3]Bonechi, C.; Tamasi, G.; Donati, A.; Bisozzi, F.; Baglioni, M.; Andreassi, M.; Ietta, F.; Leone, G.; Magnani, A,; Rossi, C.; *Biophysical Chemistry*, **2025**, 318, 0301-4622

APC - D4 - P11

One-pot multisubstrate screening for asymmetric catalysis enabled by ^{19}F NMR-based simultaneous chiral analysis

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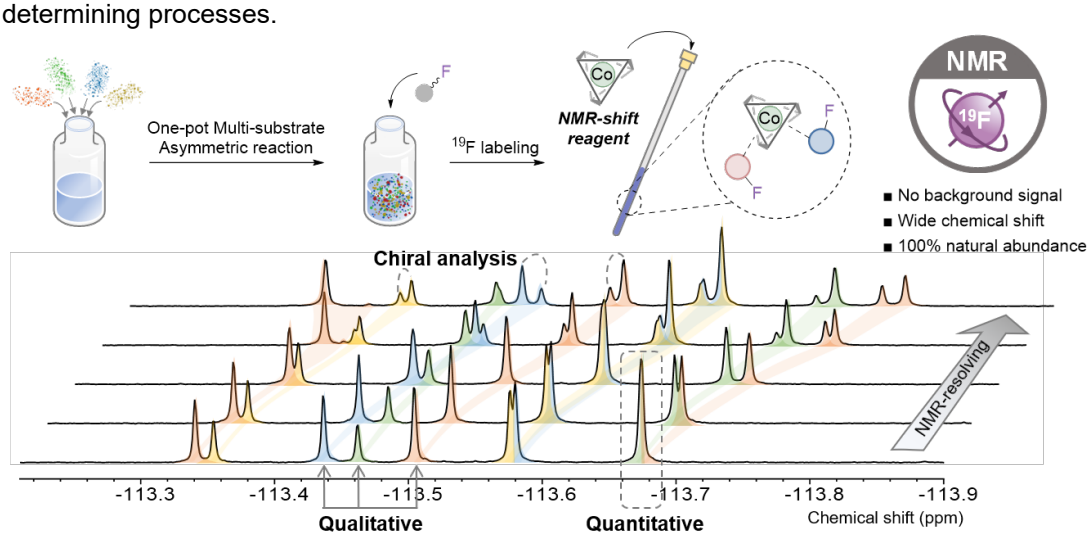
Exploring a diverse chemical space is essential for advancing asymmetric synthesis.[2] The complexity of the chirality-determining processes often requires resource-intensive optimization campaigns across multiple substrates.[3] Although one-pot multisubstrate screening offers a promising solution for high-throughput screening (HTS), a persistent challenge lies in the accurate and efficient analysis of complex reaction mixtures, which has traditionally relied on chromatography-based techniques with limited resolution.[4] In this work, we present a rapid multisubstrate screening workflow that utilizes ^{19}F NMR spectroscopy for simultaneous chiral analysis. By employing an NMR-shifting cobalt reagent, we accurately determined both yields and enantiomeric excesses for up to 21 different substrates in a single reaction mixture during the ruthenium-catalyzed asymmetric reductive amination of ketones. This method facilitates precise chiral analysis through dynamic peak shifts and splitting in ^{19}F NMR spectra induced by the shift reagent.[5] This approach accelerates the evaluation of structure-selectivity relationships, offering valuable mechanistic insights into enantio-determining processes.



Simultaneous analysis using 19F NMR spectroscopy and NMR-shift reagents

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[1]Kim, D.; Choi, G.; Kim,H. *J. Am. Chem. Soc.* **2025**, *147*, 19770-19776.
[2]Schrader, M. L.; Schafer, F. R.; Schaefers, F.; Glorius, F. *Nature Chemistry* **2024**, *16*, 491-498.
[3]Wagen, C. C.; McMinn, S. E.; Kwan, E. E.; Jacobsen, E. N. *Nature* **2022**, *610*, 680-686.
[4]Fogel, M. S.; Koide, K. *Org. Process Res. Dev.* **2023**, *27*, 1235-1247.
[5]Jang, S.; Park, H.; Duong, Q. H.; Kwahk, E.; Kim, H. *Anal. Chem.* **2022**, *94*, 1441-1446.

APC - D4 - P12

Development and validation of an LC-MS/MS method for the simultaneous determination of alprazolam, bromazepam, clonazepam, diazepam and flunitrazpam in human urine and its application to samples from suspected drug abusers

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A simple and reliable method was developed using LC-MS/MS to quantify alprazolam, bromazepam, clonazepam, diazepam, and flunitrazepam in clinical samples. This method was validated for the simultaneous determination of alprazolam, bromazepam, clonazepam, diazepam, and flunitrazepam. It was applied to human urine samples collected from people suspected of drug abuse in the Kuwaiti region. Formic acid in water and acetonitrile was used in mobile phase with a gradient mode of elution using C18 reverse-phase column. The instrument was operated in a positive mode with an electrospray ionization source using multiple reaction monitoring. For sample extraction, the liquid-liquid extraction technique was used. The method was validated for limit of detection, limit of quantitation, selectivity, linearity, accuracy, and precision. The concentration for limit of quantitation was 6.0 ng/mL, the linearity ranged from 2.0 to 300 ng/mL for each of the analytes, and the r^2 values were ≥0.99. The accuracy was found to be within a range of 80-120% and precision had a %RSD of ≤15% for each of the analytes. The method was applied to 48 urine samples collected from those suspected of drug abuse by the Toxicology Dept. of the General Dept. of Criminal Evidence, Kuwait, and alprazolam, bromazepam, clonazepam, diazepam and flunitrazepam were identified commonly in the samples. The overall drug positivity rate obtained considering 48 samples was 93.75%. Based on these results and successful determination of alprazolam, bromazepam, clonazepam, diazepam and flunitrazepam in human urine samples from those suspected of drug abuse, this method is deemed to be suitable for its routine analysis.

1. Sofalvi S., Lavins E.S., Kaspar C.K., Michel H.M., Mitchell-Mata C.L., Huestis M.A., Apollonio L.G. Development and validation of an LC–MS-MS method for the detection of 40 benzodiazepines and three Z-drugs in blood and urine by solid-phase extraction. J. Anal. Toxicol. 2020;44:708–717. doi: 10.1093/jat/bkaa072. - DOI – PubMed
2. Al-Waheeb S., Al-Omair N., Mahdi A. Patterns of drug overdose deaths in Kuwait from 2014 to 2018. Public Health Pract. 2021;2:100181. doi: 10.1016/j.puhip.2021.100181. - DOI - PMC – PubMed
3. Al-Matrouk A., Al-Hasan M., Naqi H., Al-Abkal N., Mohammed H., Haider M., Al-Shammeri D., Bojbarah H. Snapshot of narcotic drugs and psychoactive substances in Kuwait: A qualitative analysis of illicit drugs and their associated mortality in Kuwait from 2015 to 2018. BMC Public Health. 2021;21:671. doi: 10.1186/s12889-021-10705-z. - DOI - PMC – PubMed
4. Tamama K. Advances in drugs of abuse testing. Clin. Chim. Acta. 2021;514:40–47. doi: 10.1016/j.cca.2020.12.010. - DOI – PubMed
5. Saxon A.J., Calsyn D.A., Haver V.M., Delaney C.J. Clinical evaluation and use of urine screening for drug abuse. West. J. Med. 1988;149:296–303. - PMC – PubMed
6. Liu Z., Short J., Rose A., Ren S., Contel N., Grossman S., Unger S. The simultaneous determination of diazepam and its three metabolites in dog plasma by high-performance liquid chromatography with mass spectroscopy detection. J. Pharm. Biomed. Anal. 2001;26:321–330. doi: 10.1016/S0731-7085(01)00404-6. - DOI – PubMed
7. Kim D.H., Cho J.Y., Chae S.I., Kang B.K., An T.G., Shim W.S., Noh Y.S., Hwang S.J., Chung E.K., Lee K.-T. Development of a simple and sensitive HPLC-MS/MS method for determination of diazepam in human plasma and its application to a bioequivalence study. Transl. Clin. Pharmacol. 2017;25:173–178. doi: 10.12793/tcp.2017.25.4.173. - DOI - PMC – PubMed
8. Smink B.E., Brandsma J.E., Dijkhuizen A., Lusthof K.J., Gier J.J.D., Egberts A.C.G., Uges D.R.A. Quantitative analysis of 33 benzodiazepines, metabolites and benzodiazepine-like substances in whole blood by liquid chromatography-(tandem) mass spectrometry. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 2004;811:13–20. doi: 10.1016/j.jchromb.2004.03.079. - DOI – PubMed
9. Abarca R., Gerona R. Development and validation of an LC-MS/MS assay for the quantitative analysis of alprazolam, α-hydroxyalprazolam and hydrocodone in dried blood spots. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 2023;1220:123639. doi: 10.1016/j.jchromb.2023.123639. - DOI – PubMed
10. Cavedal L.E., Mendes F.D., Domingues C.C., Patni A.K., Monif T., Reyar S., Pereira A.d.S., Mendes G.D., De Nucci G. Clonazepam quantification in human plasma by high-performance liquid chromatography coupled with electrospray tandem mass spectrometry in a bioequivalence study. J. Mass Spectrom. 2007;42:81–88. doi: 10.1002/jms.1141. - DOI – PubMed
11. Kratzsch C., Tenberken O., Peters F.T., Weber A.A., Kraemer T., Maurer H.H. Screening, library-assisted identification and validated quantification of 23 benzodiazepines, flumazenil, zaleplone, zolpidem and zopiclone in plasma by liquid chromatography/mass spectrometry with atmospheric pressure chemical ionization. J. Mass Spectrom. 2004;39:856–872. doi: 10.1002/jms.599. - DOI – PubMed
12. Glover S.J., Allen K.R. Measurement of benzodiazepines in urine by liquid chromatography-tandem mass spectrometry: Confirmation of samples screened by immunoassay. Ann. Clin. Biochem. 2010;47:111–117. doi: 10.1258/acb.2009.009172. - DOI – PubMed
13. Chèze M., Villain M., Pépin G. Determination of bromazepam, clonazepam and metabolites after a single intake in urine and hair by LC-MS/MS: Application to forensic cases of drug facilitated crimes. Forensic Sci. Int. 2004;145:123–130. doi: 10.1016/j.forsciint.2004.04.066. - DOI – PubMed
14. Lee H.H., Lee J.F., Lin S.Y., Chen B.H. Simultaneous identification of abused drugs, benzodiazepines, and new psychoactive substances in urine by liquid chromatography tandem mass spectrometry. Kaohsiung J. Med. Sci. 2016;32:118–127. doi: 10.1016/j.kjms.2016.01.007. - DOI - PMC – PubMed
15. Villain M., Chèze M., Tracqui A., Ludes B., Kintz P. Windows of detection of zolpidem in urine and hair: Application to two drug facilitated sexual assaults. Forensic Sci. Int. 2004;143:157–161. doi: 10.1016/j.forsciint.2004.04.019. - DOI – PubMed
16. Kintz P., Villain M., Cirimele V., Pépin G., Ludes B. Windows of detection of lorazepam in urine, oral fluid and hair, with a special focus on drug-facilitated crimes. Forensic Sci. Int. 2004;145:131–135. doi: 10.1016/j.forsciint.2004.04.027. - DOI – PubMed

17. Marin S.J., Coles R., Merrell M., McMillin G.A. Quantitation of benzodiazepines in urine, serum, plasma, and meconium by LC-MS-MS. J. Anal. Toxicol. 2008;32:491–498. doi: 10.1093/jat/32.7.491. - DOI – PubMed
18. Jang M., Chang H., Yang W., Choi H., Kim E., Yu B.H., Oh Y., Chung H. Development of an LC-MS/MS method for the simultaneous determination of 25 benzodiazepines and zolpidem in oral fluid and its application to authentic samples from regular drug users. J. Pharm. Biomed. Anal. 2013;74:213–222. doi: 10.1016/j.jpba.2012.11.002. - DOI – PubMed
19. Arantes A.C.F., da Cunha K.F., Cardoso M.S., Oliveira K.D., Costa J.L. Development and validation of quantitative analytical method for 50 drugs of antidepressants, benzodiazepines and opioids in oral fluid samples by liquid chromatography–tandem mass spectrometry. Forensic Toxicol. 2021;39:179–197. doi: 10.1007/s11419-020-00561-8. – DOI
20. Kronstrand R., Nyström I., Josefsson M., Hodgins S. Segmental ion spray LC-MS-MS analysis of benzodiazepines in hair of psychiatric patients. J. Anal. Toxicol. 2002;26:479–484. doi: 10.1093/jat/26.7.479. - DOI – PubMed
21. Villain M., Chèze M., Tracqui A., Ludes B., Kintz P. Testing for zopiclone in hair application to drug-facilitated crimes. Forensic Sci. Int. 2004;145:117–121. doi: 10.1016/j.forsciint.2004.04.026. - DOI – PubMed
22. Villain M., Chèze M., Dumestre V., Ludes B., Kintz P. Hair to document drug-facilitated crimes: Four cases involving bromazepam. J. Anal. Toxicol. 2004;28:516–519. doi: 10.1093/jat/28.6.516. - DOI – PubMed
23. Banaszkiewicz L., Woźniak M.K., Kaliszan M., Kot-Wasik A. Determination of benzodiazepines and Z-hypnotic drugs in whole blood samples by GC–MS/MS: Method development, validation and application. Microchem. J. 2023;193:109115. doi: 10.1016/j.microc.2023.109115. – DOI
24. Perez E.R., Knapp J.A., Horn C.K., Stillman S.L., Evans J.E., Arfsten D.P. Comparison of LC-MS-MS and GC-MS analysis of benzodiazepine compounds included in the drug demand reduction urinalysis program. J. Anal. Toxicol. 2016;40:201–207. doi: 10.1093/jat/bkv140. - DOI - PMC – PubMed
25. Negrusz A., Moore C., Deitermann D., Lewis D., Kaleciak K., Kronstrand R., Feeley B., Niedbala R.S. Highly sensitive micro-plate enzyme immunoassay screening and NCI-GC-MS confirmation of flunitrazepam and its major metabolite 7-aminoflunitrazepam in hair. J. Anal. Toxicol. 1999;23:429–435. doi: 10.1093/jat/23.6.429. - DOI – PubMed
26. Cirimele V., Kintz P., Ludes B. Screening for forensically relevant benzodiazepines in human hair by gas chromatography-negative ion chemical ionization-mass spectrometry. J. Chromatogr. B Biomed. Appl. 1997;700:119–129. doi: 10.1016/S0378-4347(97)00337-X. - DOI – PubMed
27. Pirnay S., Ricordel I., Libong D., Bouchonnet S. Sensitive method for the detection of 22 benzodiazepines by gas chromatography-ion trap tandem mass spectrometry. J. Chromatogr. A. 2002;954:235–245. doi: 10.1016/S0021-9673(02)00190-5. - DOI – PubMed
28. Albishri H.M., Aldawsari N.A., Abd El-Hady D. A Simple and Reliable Liquid Chromatographic Method for Simultaneous Determination of Five Benzodiazepine Drugs in Human Plasma. Analytica. 2022;3:251–265. doi: 10.3390/analytica3020018. – DOI
29. Al-Hawasli H., Al-Khayat M.A., Al-Mardini M.A. Development of a validated HPLC method for the separation and analysis of a Bromazepam, Medazepam and Midazolam mixture. J. Pharm. Anal. 2012;2:484–491. doi: 10.1016/j.jpha.2012.05.001. - DOI - PMC – PubMed
30. Soltaninejad K., Karimi M., Nateghi A., Daraei B. Simultaneous determination of six benzodiazepines in spiked soft drinks by high performance liquid chromatography with ultra violet detection (HPLC-UV) Iran. J. Pharm. Res. 2016;15:457–463. - PMC – PubMed
31. Bell C., George C., Kicman A.T., Traynor A. Development of a rapid LC-MS/MS method for direct urinalysis of designer drugs. Drug Test. Anal. 2011;3:496–504. doi: 10.1002/dta.306. - DOI – PubMed
32. Yuan C., Chen D., Wang S. Drug confirmation by mass spectrometry: Identification criteria and complicating factors. Clin. Chim. Acta. 2015;438:119–125. doi: 10.1016/j.cca.2014.08.021. - DOI – PubMed
33. Seger C. Usage and limitations of liquid chromatography-tandem mass spectrometry (LC-MS/MS) in clinical routine laboratories. Wien. Med. Wochenschr. 2012;162:499–504. doi: 10.1007/s10354-012-0147-3. - DOI – PubMed
34. Dams R., Huestis M.A., Lambert W.E., Murphy C.M. Matrix effect in bio-analysis of illicit drugs with LC-MS/MS: Influence of ionization type, sample preparation, and biofluid. J. Am. Soc. Mass Spectrom. 2003;14:1290–1294. doi: 10.1016/S1044-0305(03)00574-9. - DOI – PubMed
35. Stokvis E., Rosing H., Beijnen J.H. Stable isotopically labeled internal standards in quantitative bioanalysis using liquid chromatography/mass spectrometry: Necessity or not? Rapid Commun. Mass Spectrom. 2005;19:401–407. doi: 10.1002/rcm.1790. - DOI – PubMed
36. Srinivas N.R. Dodging matrix effects in liquid chromatography tandem mass spectrometric assays—Compilation of key learnings and perspectives. Biomed. Chromatogr. 2009;23:451–454. doi: 10.1002/bmc.1152. - DOI – PubMed
37. Fisichella M., Odoardi S., Strano-Rossi S. High-throughput dispersive liquid/liquid microextraction (DLLME) method for the rapid determination of drugs of abuse, benzodiazepines and other psychotropic medications in blood samples by liquid chromatography-tandem mass spectrometry (LC-MS/MS) and application to forensic cases. Microchem. J. 2015;123:33–41. doi: 10.1016/j.microc.2015.05.009. – DOI
38. Kohler I., Schappler J., Sierro T., Rudaz S. Dispersive liquid-liquid microextraction combined with capillary electrophoresis and time-of-flight mass spectrometry for urine analysis. J. Pharm. Biomed. Anal. 2013;73:82–89. doi: 10.1016/j.jpba.2012.03.036. - DOI – PubMed
39. Saraji M., Khalili Boroujeni M., Hajialiakbari Bidgoli A.A. Comparison of dispersive liquid-liquid microextraction and hollow fiber liquid-liquid-liquid microextraction for the determination of fentanyl, alfentanil, and sufentanil in water and biological fluids by high-performance liquid chromatography. Anal. Bioanal. Chem. 2011;400:2149–2158. doi: 10.1007/s00216-011-4874-x. - DOI – PubMed
40. Shamsipur M., Fattahi N. Extraction and determination of opium alkaloids in urine samples using dispersive liquid-liquid microextraction followed by high-performance liquid chromatography. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 2011;879:2978–2983. doi: 10.1016/j.jchromb.2011.08.033. - DOI – PubMed
41. Ahmadi-Jouibari T., Fattahi N., Shamsipur M. Rapid extraction and determination of amphetamines in human urine samples using dispersive liquid-liquid microextraction and solidification of floating organic drop followed by high performance liquid chromatography. J. Pharm. Biomed. Anal. 2014;94:145–151. doi: 10.1016/j.jpba.2014.01.044. - DOI – PubMed
42. Mercieca G., Odoardi S., Cassar M., Strano Rossi S. Rapid and simple procedure for the determination of cathinones, amphetamine-like stimulants and other new psychoactive substances in blood and urine by GC–MS. J. Pharm. Biomed. Anal. 2018;149:494–501. doi: 10.1016/j.jpba.2017.11.024. - DOI – PubMed
43. European Monitoring Centre for Drugs and Drug Addiction . European Drug Report 2019: Trends and Developments. Publications Office of the European Union; Luxembourg: 2019. [(accessed on 17 July 2025)]. Available online: https://www.narkotik.pol.tr/kurumlar/narkotik.pol.tr/TUB%C4%B0M/Uluslar-....
44. International Conference on Harmonization of Technical Requirement for Registration of Pharmaceuticals for Human Use, Validation of Analytical Procedure: Text and Methodology Q2(R1); European Medicines Agency: Geneva, Switzerland. 2005. [(accessed on 14 September 2023)]. Available online: https://www.ema.europa.eu/en/documents/scientific-guideline/ich-guidelin...
45. Fraser A.D. A 6-year experience with urine drug testing by family service agencies in Nova Scotia, Canada. Forensic Sci. Int. 2001;121:151–156. doi: 10.1016/S0379-0738(01)00398-X. - DOI - PubMed

The 10th EuChemS Chemistry Congress

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

CAI - D4 - P01
Model order reduction of CFD model for membrane distillation

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Membrane distillation (MD) is an emerging process for purifying water solutions using low grade heat such as waste heat or solar thermal energy. Optimization of membrane distillation is critical for optimal production and its viability for industrial use. Theoretical approaches such as numerical modeling of chemical processes can predict the system behavior and inhibited performance such as lower mass flux due to concentration and temperature polarization. Simulations can give insight to processes and provide data of hard to measure properties such as membrane surface temperature. Computational fluid dynamics (CFD) simulation is widely accepted as a tool for process simulations. The complex setup of CFD and high computational cost are needed for a simulation. To decrease the high computational cost, a model order reduction numerical simulation and machine learning (ML) model were made to calculate the mass flux through the membrane region. A direct-contact MD module process was simulated using CFD and model order reduction in-house Python code was created to simulate the temperature inside the MD module. The reduced-order model was validated against CFD and experimental data, indicating similar performance in predicting the mass flux. A trained neural network provided a data-driven prediction method for mass flux in a DCMD module. The results show that model order reduction and data-driven approaches can predict the mass flux with high prediction accuracy, offering simpler performance prediction with a lower computational cost.

[1]Thajudeen, K. Y.; Ahmed, M. M.; Alshehri, S. A. *Sci. Rep.* **2024**, *14*(1), 23970.
[2]Johnston, J.; Dischinger, S. M.; Nassr, M.; Lee, J. Y.; Bigdelou, P.; Freeman, B. D.; Gleason, K. L.; Martinand, D.; Miller, D. J.; Molins, S.; Spycher, N.; Stringfellow, W. T.; Tilton, N. *J. Membr. Sci.* **2023**, *675*, 121508.

CAI - D4 – P02

Cross-validated screening of natural products targeting two distinct functional sites of the bacterial ribosome: An in-silico study

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The World Health Organization identifies antibiotic resistance as a critical global health threat, necessitating the development of novel therapeutic strategies [1]. The bacterial ribosome is one of the primary targets for antibiotic development due to its vital role in protein synthesis, specifically within the decoding center (DC) and peptidyl-transferase center (PTC) [2]. Natural products represent superior alternatives to traditional synthetic libraries, as they possess higher sp^3 carbon content, richer hydrogen bonding profiles, and lower toxicity risks [3]. This study explores natural product candidates targeting DC and PTC regions of the *E. coli* ribosome. In this research, an integrated collection of natural product libraries was screened against these ribosomal sites. The computational workflow was validated through redocking crystallographic ligands using Glide [4] and AutoDock Vina [5]. Following docking, binding affinities were refined using Prime MM-GBSA. To prioritize candidates, refined hits underwent rigorous filtering, including substructure analysis, ADME property evaluation, and fingerprint-based clustering to ensure chemical diversity and drug-likeness. Structural behavior was evaluated through three independent 100 ns replica MD simulations, where trajectories were analyzed to assess molecular interaction persistence and binding free energies. This multilayered approach identified promising natural products with high affinity and stability, establishing a robust discovery workflow.

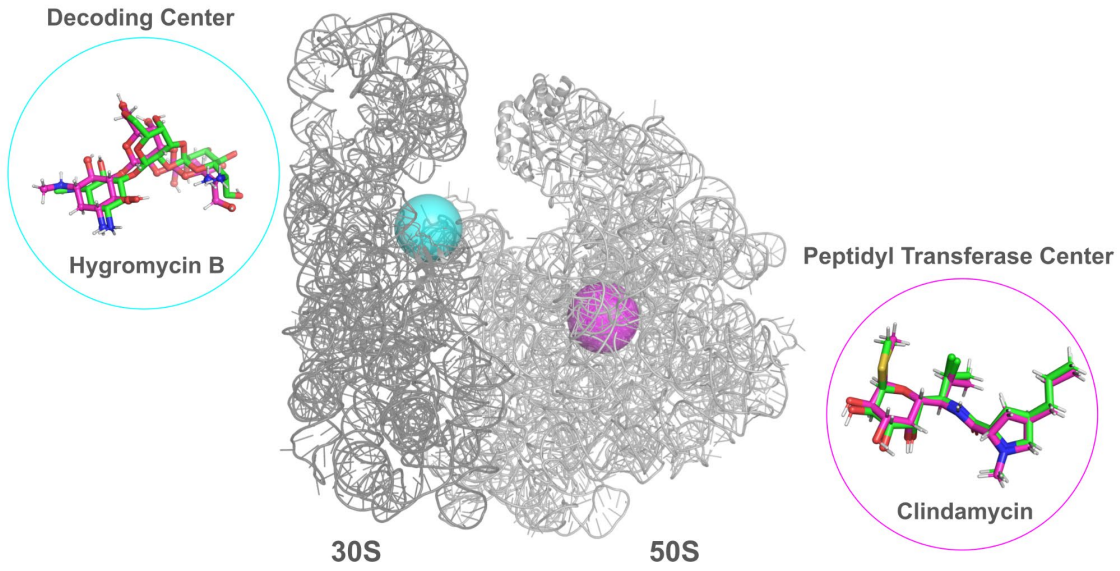

Fig. 1. 3D structure of *E.coli* 70S ribosome (crystal pose: green, best docking pose: magenta).

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[1]World Health Organization. Global action plan on antimicrobial resistance; World Health Organization: Geneva, Switzerland, 2015.
[2]Wilson, D. N. Nat. Rev. Microbiol. 2014, 12, 35–48.
[3]Atanasov, A. G.; Zotchev, S. B.; Dirsch, V. M.; Supuran, C. T. Nat. Rev. Drug Discov. 2021, 20, 200–216.
[4]Halgren, T. A.; Murphy, R. B.; Friesner, R. A.; Beard, H. S.; Frye, L. L.; Pollard, W. T.; Banks, J. L. J. Med. Chem. 2004, 47, 1750–1759.
[5]Trott, O.; Olson, A. J. J. Comput. Chem. 2010, 31, 455–461.

CAI - D4 - P03
Beyond bulk aggregation: Interfacial chloride recognition by triazolophane on graphene

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Anion recognition and capture are central to sensing, separation, and remediation, yet they remain difficult in water because hydration and receptor aggregation often suppress binding. Triazolophanes provide a useful model for this problem because their rigid frameworks and polarized C–H groups support anion recognition while remaining structurally tunable. Here, we combined atomistic molecular dynamics simulations and free-energy calculations to investigate how solvent environment and surface confinement affect chloride capture by triazolophane macrocycles, including both the parent host and an alkyl-substituted derivative, in water and organic solvents, both in bulk solution and at a graphene interface.
Comparison of the parent triazolophane with its alkyl-substituted derivative shows that hydrophobic substitution has only a limited effect in bulk solution but becomes more important at the interface, where the modified receptor adsorbs more strongly on graphene and forms more stable interfacial assemblies. Solvent then emerges as a second key factor: as the number of macrocycles increases, it strongly influences the access to the macrocycle cavity and the extent of supramolecular self-assembly. In water, hydrophobic aggregation limited chloride binding efficiency, whereas in organic solvents, the receptor cavity remains more accessible to the anion. At the graphene interface, however, this tendency changes, making chloride capture more favorable.
Overall, these results highlight interfacial confinement as a useful element in the design of surface-assisted anion-capture systems and provide a basis for developing responsive supramolecular materials for aqueous ion recognition.

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CAI - D4 - P04

Balancing data quantity and quality: Evaluating curation strategies for bioactivity prediction

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Building good machine-learning (ML) models to predict the bioactivity of novel chemical matter remains a challenging task. Accurate models require a training set with a large number of diverse compounds and a low level of noise. When extracting data from public databases such as ChEMBL, different levels of curation rigor may be applied, resulting in training sets of varying size, diversity, and, presumably, noise levels. It is not possible to know a priori whether increasing the size of the dataset at the cost of adding more noise improves model generalization. To assess this trade-off, we compare three data curation and modeling approaches: (1) models trained on data for a single target, (2) models trained on target-specific data further restricted to a single set of assay conditions, and (3) multitask learning (MTL) models where each assay condition is treated as a separate task. This MTL approach was designed to bridge the gap between data quantity and quality. Graph neural networks (GNN) and random forests (RF) regressors are evaluated via a leave-assay-out strategy to minimize noise in the test sets. Our results show no meaningful performance differences between these curation strategies, suggesting that for lead-optimization tasks, increasing data quantity at the expense of label consistency does not improve generalization. Notably, the MTL approach also failed to provide a performance advantage. Additionally, we find that GNNs exhibit high seed-dependent variability in connection with the comparatively small training sets common for bioactivity measurements, highlighting the necessity of multi-seed evaluation for robust model assessment.

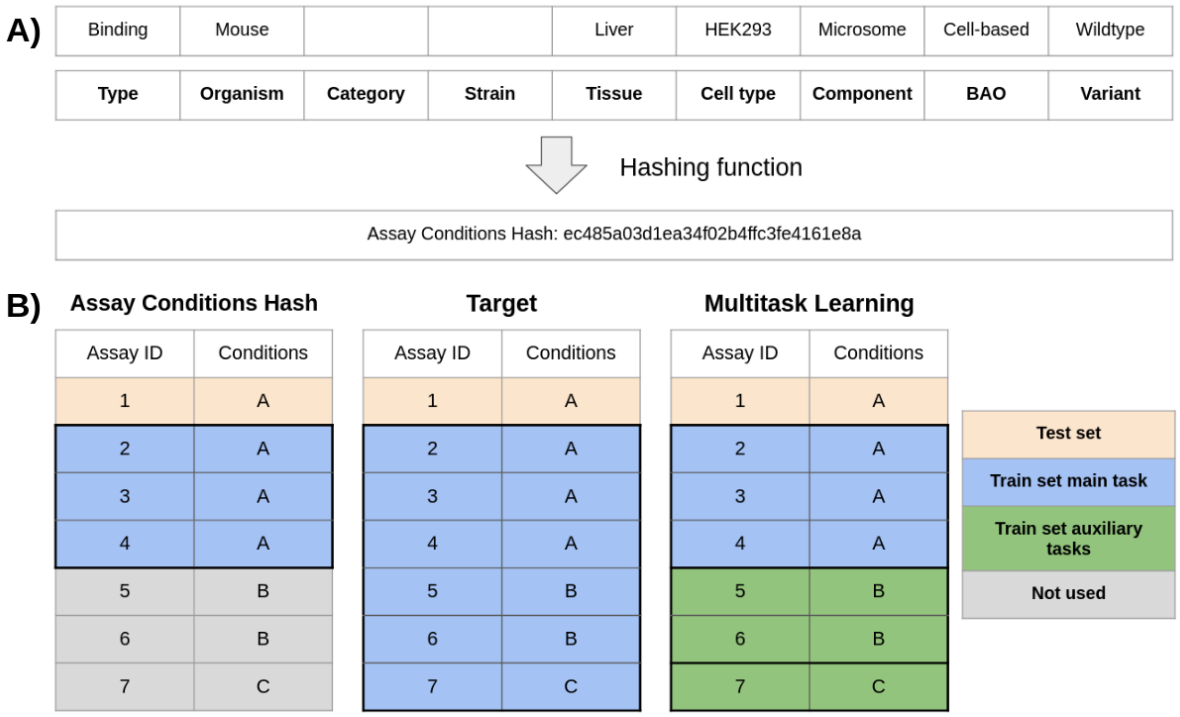

Fig. 1. (**A**): Hashing of assay metadata into the assay conditions hash (ACH). (**B**): Schematic visualization of the curation strategies ACH (left), target (middle), and MTL (right) and the corresponding data splitting. All models are evaluated on the same test set, i.e., in the example assay 1 with conditions A. For ACH, a model is trained on assays 2-4 with the same assay conditions as the test set (conditions A). For target curation, a model is trained on assays 2-7 with mixed assay conditions (conditions A-C). For MTL, a model is trained for three tasks simultaneously (tasks A, B, and C), representing prediction of bioactivity under different assay conditions. Only predictions for the task with conditions corresponding to the test set (condition A) are evaluated on the test set.

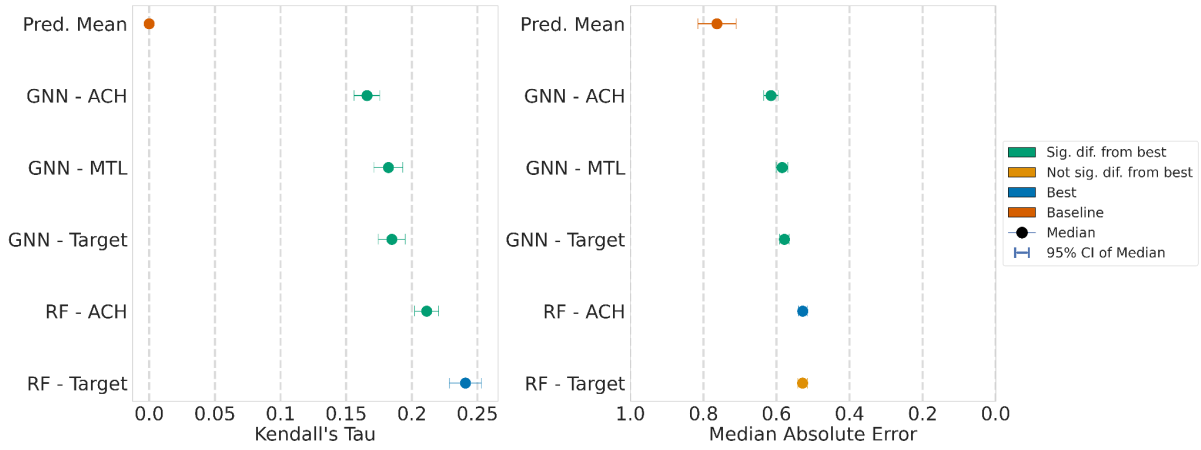

Fig. 2. Comparison of the performance of the ML models over the 422 test sets. The best method is determined based on the best median value of the performance metric. All other methods are compared to this best method using the Conover-Friedman post hoc test with Bonferroni correction for multiple comparisons ($\alpha = 0.05$) as implemented in scikit-posthocs. Performance is put in context of predicting the mean of the (target) training set. Left: Kendall's τ, right: median absolute error (medAE).

[1]Landrum, G. A., Riniker, S., Combining IC50 or K i Values from Different Sources Is a Source of Significant Noise. Journal of Chemical Information and Modeling., **2024**, 64, 5, 1560–1567, 10.1021/acs.jcim.4c00049
[2]Zdrazil, M., *et al*., The ChEMBL Database in 2023: a drug discovery platform spanning multiple bioactivity data types and time periods. Nucleic acids research., **2024**, 52, D1, D1180-1192, 10.1093/nar/gkad1004

CAI - D4 - P05

Unified data-driven flow regime identification in horizontal and vertical multiphase pipe flows using dynamic pressure signals

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Flow regime identification is essential for the reliable operation of gas–liquid multiphase systems widely encountered in chemical and process industries. However, real-time monitoring remains challenging in industrial pipelines where direct visualization is not feasible. In this work, a unified, data-driven framework is developed for flow regime classification in both horizontal and vertical pipe systems using dynamic pressure signals. Dynamic pressure signals are processed using Discrete Wavelet Transform (DWT) to extract multiscale features that capture the underlying flow dynamics. To enable interpretable data representation, multiple dimensionality reduction techniques are evaluated, with Kernel Fisher Discriminant Analysis (KFDA) providing optimal clustering and visualization of flow regimes in a reduced feature space. Machine learning models were then evaluated using an AutoML workflow to identify the best-performing classifier. The proposed methodology is first validated independently for horizontal and vertical flows, achieving testing accuracies of 92.5% and 90.2%, respectively. Building on this, a unified model is developed by integrating both configurations into a single framework. The optimal pipeline (DWT–KFDA–ANN) achieves 100% training accuracy and 92.5% testing accuracy while maintaining strong generalization across flow orientations. The resulting virtual flow regime maps enable direct projection of new pressure data, supporting real-time classification using a moving-window approach. By combining signal processing with interpretable machine learning, this work demonstrates the potential of data-driven methodologies for monitoring and decision support in complex multiphase systems relevant to chemical and energy applications.

Keywords: Two-phase flow; flow regime identification; dynamic pressure; machine learning; AutoML; dimensionality reduction; industrial process monitoring

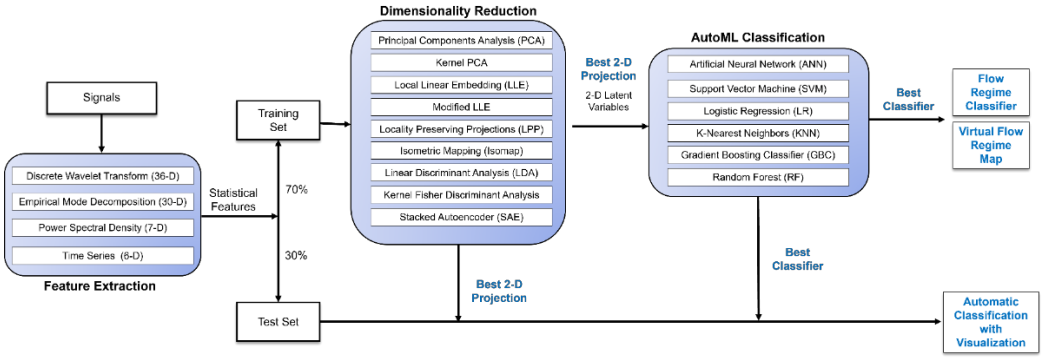

Fig. 1. Overview of the proposed data-driven workflow for flow regime identification. Dynamic pressure signals are processed through feature extraction (DWT), dimensionality reduction (KFDA), and AutoML-based classifier selection to generate a virtual flow regime map for automated classification.

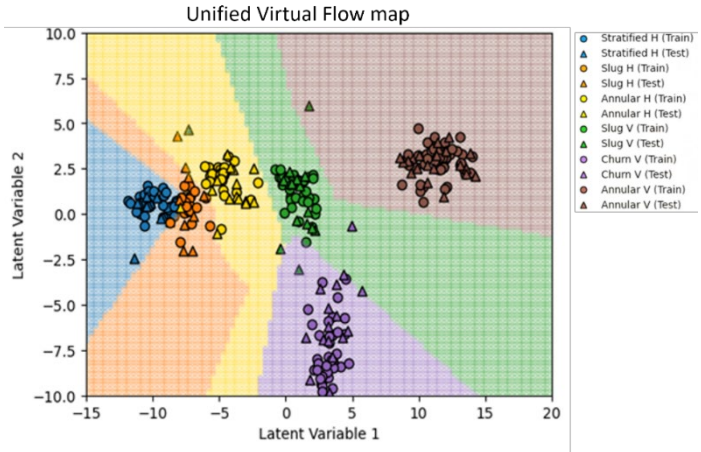

Fig. 2. Unified virtual flow regime map obtained using KFDA-based dimensionality reduction and ANN classification. Data from both horizontal and vertical pipe configurations form distinct clusters with clear decision boundaries, demonstrating the generalization capability of the proposed data-driven framework.

The 10th EuChemS Chemistry Congress

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Chemistry Meets Biology & Food Science (CBF)

CBF - D4 - P01
High-resolution mass spectrometry: Unlocking the chemical complexity of xylem sap

Maria Assunta Crescenzi[1,2], Zeinab Hamouche[2,3,] Vincenzo Verrastro[3], Erica Tinelli[2], Daniele Cornara[2], Paola Montoro[1]
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Mass spectrometry (MS) is a powerful analytical tool for the comprehensive characterization of xylem sap, offering exceptional sensitivity, specificity, and the ability to detect a broad spectrum of metabolites, from primary to secondary metabolism-related compounds. High-resolution MS (HR-MS) further enhances these capabilities, enabling precise mass measurements, robust molecular formula assignment, structural elucidation, and the identification of metabolites in biological matrices even at trace concentrations [1]. Untargeted HR-MS approaches facilitate the discovery of novel biomarkers and metabolic patterns that are otherwise inaccessible with conventional techniques. Applications of this technology include the investigation of plant responses to abiotic stress, the characterization of the molecule(s) underlying plant–herbivore interaction, and the evaluation of environmental drivers shaping xylem chemistry [2]. A particularly innovative application is the study of xylem sap composition in relation to host plant acceptance and colonization by xylem-sap feeding insects, such as *Philaenus spumarius* (also known as the meadow spittlebug), the main European vector of *Xylella fastidiosa* ST53 to olive plants [3]. In the present study, xylem sap samples from several *Olea europaea* varieties were profiled using an untargeted metabolomics workflow to identify metabolites potentially associated with acceptance or rejection by *P. spumarius*. The metabolites detected predominantly belong to the chemical classes of organic acids, amino acids, sugars, terpenes, and phenolic compounds, which were subsequently selected for targeted quantitative analysis. Collectively, this study represents the first comprehensive characterization of xylem sap metabolites mediating spittlebug-olive interaction, and successive pathogen transmission. Additionally, the results lay the groundwork for the selection of potentially resistant germplasm and the development of agronomic strategies aimed at reducing host plant suitability for the vector, thereby contributing to the containment of pathogen spread.

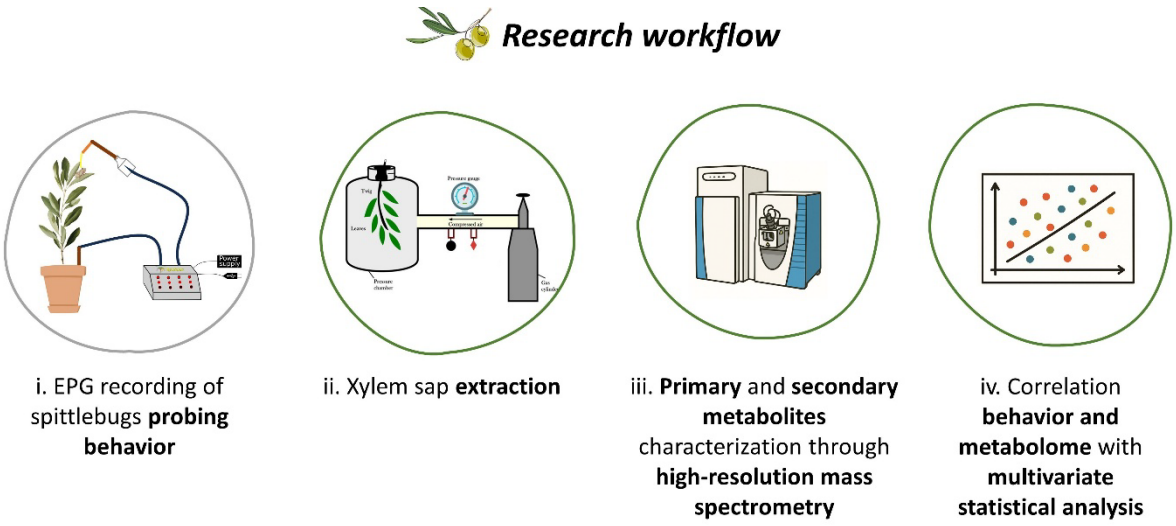

Fig. 1. Experimental workflow illustrating EPG-based recording of spittlebug feeding behaviour, xylem sap extraction, high-resolution mass spectrometry–based metabolomic profiling, and multivariate analysis integrating behavioural and chemical data.

[1]Rathahao-Paris, E., Alves, S., Junot, C. et al. *Metabolomics*. **2016**, *12*, 10.
[2]Sun, J.; L,Q.; Xu, H.; Zhang, W. *Metabolites*. **2022**, *12(4)*:361.
[3]Cornara, D.; Zaffaroni-Caorsi, V.; Hamouche, Z.; et al. *J Pest Sci.* **2024**; 97: 1-13.

CBF - D4 - P02

Stability meets mobility: *N*-heterocyclic carbene-based tethers for functional biomimetic membranes

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Biological membranes exhibit extraordinary structural and functional complexity, making simplified model systems essential for understanding individual membrane components and processes. Tethered bilayer lipid membranes (tBLMs) provide a powerful platform for such studies. However, conventional thiol-based anchors have a limited lipid mobility and stability under ambient conditions.[1–3]

Here, we present the design, synthesis and characterization of novel *N*-heterocyclic carbene (NHC)-based tethered bilayer lipid membranes assembled in gold substrate as stable alternative to currently used systems with an optimized surface density and increased mobility.[4]

Self-assembled monolayer (SAM) formation was achieved under mild conditions[5] using triflate NHC precursors and surface density was systematically tuned through a variation of *N,N*-substituents.[6] Successful SAM formation was confirmed by contact angle measurements, cyclic voltammetry and X-ray photoelectron spectroscopy (XPS).

To assess the applicability of NHC-based SAMs for membrane model systems, lipid bilayers were formed using vesicle fusion with commercially available lipids. Electrochemical impedance spectroscopy (EIS) was employed to test bilayer formation and functional performance, and results were compared to conventional thiol-tethered systems.

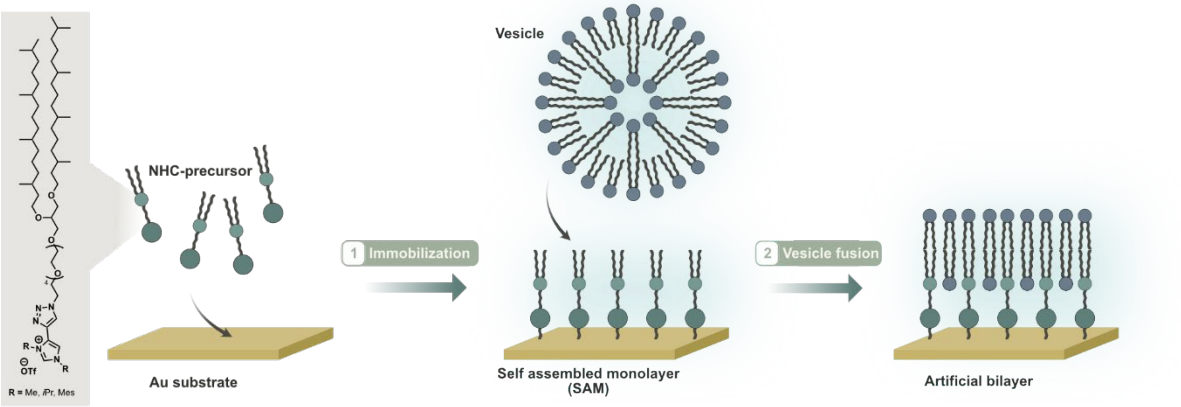

Fig. 1. Formation of (1) a self-assembled monolayer (SAM) using NHC-triflate salt precursors and (2) an artificial bilayer using vesicle fusion

[1]Schlenoff, J. B.; *J. Am. Chem. Soc.* **1995**, *117* (50), 12528–12536.
[2]Schoenfisch, M. H.; *J. Am. Chem. Soc.* **1998**, *120* (18), 4502–4513.
[3]Flynn, N. T.; *Langmuir* **2003**, *19* (26), 10909–10915.
[4]Wang, G.; *Nat. Chem.* **2017**, *9* (2), 152–156.
[5]Crudden, C. M.; *Nat. Commun.* **2016**, *7* (1), 12654.
[6]Lovat, G.; *Chem Sci* **2019**, *10* (3), 930–935.

CBF - D4 - P03

Effect of Noscapine Hydrochloride on the near-infrared optical properties of Indocyanine Green

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Indocyanine Green (ICG) is an FDA-approved near-infrared fluorophore widely utilized in biomedical imaging and photothermal therapy. However, its clinical applicability is limited by poor stability, rapid degradation, and concentration dependent aggregation. In this study, we report for the first time the role of Noscapine hydrochloride (Np·HCl), a benzyl isoquinoline alkaloid with established anticancer properties, in modulating the optical and therapeutic characteristics of ICG through controlled aggregation. Spectroscopic investigations revealed that Np·HCl promotes intermolecular aggregation of ICG at micromolar concentrations. Absorption studies demonstrated concentration dependent spectral shifts and intensity variations, indicating the coexistence of H- and J-type aggregates. Gaussian deconvolution of absorption spectra confirmed redistribution of monomer and aggregate populations, with the appearance of new near-infrared band (~835 nm) signifying J-aggregate formation. Fluorescence measurements showed progressive quenching of ICG emission with increasing Np·HCl concentration, supported by Stern Volmer analysis suggesting combined static and dynamic quenching mechanisms. Stability studies demonstrated enhanced resistance of ICG towards photodegradation and long-term storage upon complexation with Np·HCl. Zeta potential and dynamic light scattering analysis confirmed the formation of stable nano-aggregates, attributed to electrostatic interactions between protonated noscapine and sulfonate groups of ICG, facilitating π-π stacking of chromophores. Further, *in vitro* cytotoxicity studies against H1299 lung adenocarcinoma cells showed dose-dependent anticancer activity. The ICG:Np·HCl combination exhibited significantly enhanced cytotoxicity with IC_{50} values of 354.4 μM and 165.8 μM for ICG and Np·HCl, respectively, demonstrating synergistic therapeutic effects. These findings highlight a novel dye-drug assembly strategy that improves both optical stability and anticancer efficacy, offering potential applications in combined chemo-photothermal therapy.

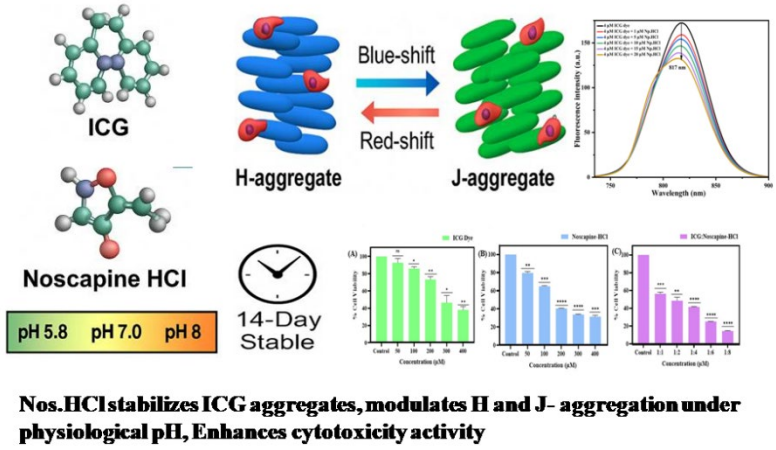

Fig. 1: Graphical abstract

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[1]Li, J.; Tian, S.; Zhang, X.; Deng, X.; Xu, H.; Yan, L. *Biomater. Sci.* **2025**, 4321–4357.
[2]Gamage, R. S.; Smith, B. D. *Chem. Biomed. Imaging* **2024**, 2 (5), 384–397.
[3]Wu, M.; Li, Z.; Yao, J.; Shao, Z.; Chen, X. *ACS Biomater. Sci. Eng.* **2019**, 5 (9), 4799–4807.

CBF - D4 - P04

Lead-silica interactions in food additive E551: Concentration-dependent effects on surface charge and colloidal stability

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With advances in nanotechnology, the use of nanomaterial-based food additives has increased, improving food quality and functionality. However, this trend also raises concerns about potential interactions between these additives and co-occurring chemical contaminants in food and water. Such interactions may modify properties, including particle size, structure, morphology and surface characteristics (Figure 1), and therefore influence the nanoparticles (NPs) behaviour and bioavailability.

In this study, developed within the MixIng-Tox project (2022.03491.PTDC), we investigated how lead (Pb) affects the physicochemical properties of the silica-based food additive E551. Four experimental scenarios were tested by combining two E551 concentrations (300 and 3000 mg·kg^{-1}) with two Pb^{2+} concentrations (1.0 and 3.0 mg·kg^{-1}).

Stable suspensions of the silica-based food additive E551were prepared using the Nanogenotox procedure and characterised using dynamic light scattering (DLS), zeta potential measurements and electron microscopy. At low E551 concentration (300 mg·kg^{-1}), Pb^{2+} decreased the magnitude of the zeta potential, consistent with partial charge neutralisation, while hydrodynamic size and polydispersity index (PdI) showed no clear concentration-dependent trend. In contrast, at high E551 concentration (3000 mg·kg^{-1}), the zeta potential remained strongly negative and was not measurably affected by Pb^{2+}. This behaviour mirrors our previous observations for Cd^{2+}.

Overall, our results reveal a concentration-dependent interplay between E551 and Pb^{2+} governed primarily by surface charge and ionic interactions. Mechanistic understanding of these processes is essential for realistic assessments of nanomaterial stability and behaviour in complex food matrices, supporting more accurate evaluations of dietary exposure and risk arising from both nanomaterial additives and co-existing chemical contaminants.

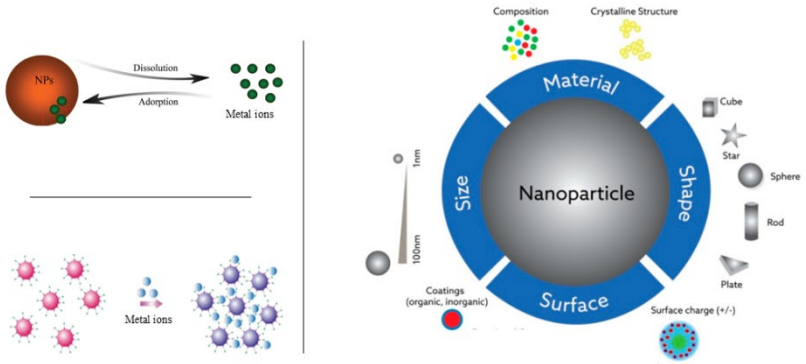

Fig.1. Possible interactions between metal ions and nanoparticles, and key NPs properties.

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CBF - D4 - P05
Effect of drying methods and pretreatments on the carbohydrate profile of Pingo de Mel figs

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Figs are widely consumed globally due to their appealing taste and high sugar content, which provides a valuable energy source [1]. While figs are traditionally dried whole, pretreatments applied before dehydration not only accelerate the drying process but also enhance product quality [2]. Despite this knowledge, no previous studies have examined how pretreatment affects the carbohydrate profile of figs. This study investigated the influence of different drying conditions on carbohydrate composition and extractability in the "Pingo de Mel" fig variety.
"Pingo de Mel" figs were dried in a solar dryer at 50 °C using three methods: whole figs without pretreatment, blanched figs in hot water, and halved figs. Sequential extraction with ethanol and water (cold and hot) yielded three soluble fractions (snAIR, CWE, and HWE) and one insoluble residue (WIR). Commercial sun-dried figs from local farmers served as controls. Carbohydrate profiles were characterized using Gas Chromatography coupled with Flame Ionization Detection (GC-FID), while uronic acids were quantified spectrophotometrically.
Results showed that although all samples had similar total sugar content, drying conditions significantly affected the sugar profile, particularly increasing solubilized pectic polysaccharide levels. Uronic acid was the major carbohydrate, reaching 82% and 70% in the CWE of halved and blanched figs, respectively, an increase by more than 1.2-fold over whole figs (62%). These fractions along with the HWE exhibited increased arabinose, xylose, and mannose levels. The elevation of arabinose and xylose suggests enhanced solubilization of pectic polysaccharides with arabinan side chains. The WIR fraction contained glucose, xylose, galactose, and arabinose, indicating the presence of xyloglucans which were also detected in higher amounts in pretreated samples.
Overall, pretreatment influenced the carbohydrate composition of "Pingo de Mel" figs by favoring the solubilization of pectic polysaccharide, suggesting its potential application for improving the extractability of these cell wall polysaccharides.

Keywords: Fig, carbohydrates, polysaccharides, pretreatment, drying.

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[1]B.R. Henriques, et al.. *Antioxidants (Basel).* **2025** Mar 19;14(3):362. doi: 10.3390/antiox14030362
[2]R. Khiari, et al. *Food Reviews International,* **2019** 35(3), 246-298. doi: 10.1080/87559129.2018.1517264

CBF - D4 - P06

The effect of processing technology on the content of acrylamide, amino acids, and reactive dicarbonyl compounds formed during bread baking

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Thermal processing and long-term storage of food initiate complex chemical reactions between carbonyl groups of reducing sugars and amino groups of amino acids, peptides, and proteins. This set of reactions, known as the Maillard reaction, is responsible for desirable flavor, aroma, and color formation, but also for the generation of potentially harmful compounds such as acrylamide and reactive dicarbonyls, including methylglyoxal (MGO) and glyoxal (GO). Free asparagine is recognized as a key precursor in acrylamide formation, and its concentration in cereal raw materials may significantly influence acrylamide levels in processed foods.

The present study aimed to evaluate the content of amino acids and Maillard reaction products in model bakery products obtained from two oat varieties (spring and winter) and to determine the effect of baking parameters on their formation. Breads were prepared under two baking conditions (200°C/90 min and 180°C/120 min). The content of amino acids (Asn, Asp, Gln, Glu), acrylamide, and reactive dicarbonyls (MGO, GO) was determined using previously developed HPLC and LC-MS methods.

Spring oat grain contained approximately twice the level of the analyzed amino acids compared to winter oat; however, this difference was not reflected in the final bread products. Baking parameters significantly affected acrylamide and carbonyl compound formation. Lower temperature combined with extended baking time reduced their levels, whereas increasing temperature and time resulted in a twofold rise in acrylamide content and a fourfold increase after parameter modification in breads from both oat varieties. No significant varietal effect on the analyzed compounds was observed.

The results confirm that time and temperature are critical determinants of Maillard reaction product formation in fresh bread, while further characterization of oat varieties may support the development of improved cereal-based products.

Acknowledgments: This contribution was supported by COST Action CA21149 (Reducing acrylamide exposure of consumers by a cereals supply-chain approach targeting asparagine (ACRYRED); https://acryred.eu/)

CBF - D4 - P07

Mining for novel tryptophanase A: extremophilic organisms *Ardenticatena maritima* and *Haloarcula japonica* as alternative to *E. Coli* in the synthesis of tryptophan analogues

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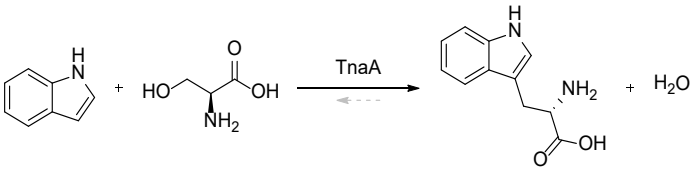
L-Tryptophan is a key amino acid with significant roles in both biological systems and pharmaceutical industries. Beyond its natural role in cellular metabolism, L-tryptophan derivatives and other non-canonical amino acids (ncAAs) are increasingly valued in medicinal chemistry and synthetic biology, contributing to the design of chemical probes and pharmaceutical scaffolds.[1,2] The biosynthesis of L-tryptophan is classically mediated by the heterodimeric tryptophan synthase (TrpS)[3], however, in *Escherichia coli* strains, it has also been well-documented that L-tryptophan can be synthesized under high concentrations of L-serine via tryptophanase A (*Ec*TnaA), an enzyme typically involved in L-tryptophan catabolism (Figure 1).[4]

Scheme 1. Biosynthesis of L-tryptophan from indole and L-serine.

This research focuses on the characterization of two novel TnaA enzymes: *Am*TnaA from the thermophilic organism *Ardenticatena maritima*[5] and *Hj*TnaA from the halophilic organism *Haloarcula japonica*.[6] Owing to their resilience under harsh physicochemical conditions, these enzymes represent promising biocatalytic tools for challenging synthetic applications, and the exploration of their substrate scope further highlights their potential for sustainable production of tryptophan derivatives and pharmaceuticals.



[1] D. K. Romney, J. Murciano-Calles, J. E. Wehrmüller and F. H. Arnold, J. Am. Chem. Soc., **2017**, 139, 10769–10776.
[2] S. Xiao, Z. Wang, B. Wang, B. Hou, J. Cheng, T. Bai, Y. Zhang, W. Wang, L. Yan and J. Zhang, Front. Microbiol., **2023**, 14, 1099098.
[3] A. R. Buller, S. Brinkmann-Chen, D. K. Romney, M. Herger, J. Murciano-Calles and F. H. Arnold, Proc. Natl. Acad. Sci. U. S. A., **2015**, 112, 14599–14604.
[4] W. A. NEWTON and E. E. SNELL, Proc. Natl. Acad. Sci. United States, **1964**, 51, 382–389.
[5] S. Kawaichi, N. Ito, R. Kamikawa, T. Sugawara, T. Yoshida and Y. Sako, Int. J. Syst. Evol. Microbiol., **2013**, 63, 2992–3002.
[6] K. Horikoshi, R. Aono and S. Nakamura, Experientia, **1993**, 49, 497–502.

CBF - D4 - P08

Implementation and optimization of automated computer processing tools for a bi-instrumental systematic toxicological analysis strategy using HPLC-DAD and GC-MS

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To modernize the laboratory's bi-instrumental Systematic Toxicological Analysis (STA) strategy, automated post-analytical interpretation tools were implemented and optimized to enhance performance, reduce time, and improve efficiency in identifying unknown toxic substances in biological samples.

Two analytical techniques, HPLC-DAD and GC-MS, were employed alongside acetylation and silylation derivatization methods. For post-analytical interpretation, Empower 2 software with the "Toxicol" library was used for HPLC-DAD data, while AMDIS combined with NIST-MS-Search and custom libraries (MPW5e, Forensic_Toxicology_V2, W11N17) supported GC-MS analysis. Calibration for Retention Indices (RI) was applied to AMDIS.

Three sets of processing parameters were defined for each chromatographic method and evaluated using chromatograms from mixtures of analytical standards. Data compilation and visualization were performed using Microsoft Excel, and MS reference libraries were modified with OpenChrom and Lib2NIST.

Empower 2's library contains 1,087 UV spectra, AMDIS uses a custom library of 11,103 MS spectra, and NIST-MS-Search accesses over 1.25 million reference MS spectra. Calibration of AMDIS for RI was successful. Detected compounds were organized by instrument and derivatization method.

Performance evaluation considered the number of compounds identified and the time required for interpretation.

Manual interpretation by an experienced toxicologist takes 30 to 40 minutes, whereas Empower 2 reduces this to 55 seconds and AMDIS to 2 minutes 30 seconds. This significant time saving facilitates routine and emergency toxicological analyses. Despite automation, expert review remains essential to ensure accuracy and reliability.

The integration of optimized automated tools for bi-instrumental STA notably enhances laboratory efficiency, enabling rapid and reliable toxicological identification while maintaining critical expert oversight.

[1]Empower Software Data Acquisition and Processing Theory Guide. 2002.
[2]PDA Software Getting Started Guide. 1997.
[3]Waters Corporation: The Science of What's Possible [Internet]. [cited 2024 Jan 16]. https://www.waters.com/nextgen/fr/fr.html
[4]Arcy PD', Mallard WG. AMDIS-USER GUIDE. 1977
[5]Amdis.net [Internet]. [cited 2024 Jan 16]. http://www.amdis.net/
[6]Chemdata:nistlibs. [cited 2024 Jan 16]. https://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:nistlibs&redirect=1

CBF - D4 - P09
Membrane organoid chips for programmable growth of stem cells

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Organoid research faces challenges in controlling microenvironmental factors and modelling complex tissue interactions. Porous membrane-based organoid chips may overcome these limitations as they potentially provide a defined 3D environment with adjustable signal gradients across a semipermeable nanoporous membrane, enabling precise control of organoid culture conditions. This approach is expected to improve organoid homogeneity and enable statistically reliable high-throughput screening. Porous membrane-based organoid chips are, therefore, a promising tool for the further development of basic organoid research and for applications in drug discovery. [1, 2] Here, we present initial results regarding the development of topographically patterned membrane-based organoid chips consisting of the block copolymer polystyrene-block-poly(vinylpyridine) (PS-*b*-P2VP). The chips' hierarchical architecture comprises topographical niches generated by replication moulding to accommodate stem cells, cell clusters and organoids as well as continuous mesopore systems generated by selective swelling-induced pore formation [3] for the transport of medium to the niche bottoms. The fabrication of spongy mesoporous PS-*b*-P2VP monoliths containing mesopore systems as well as topographic niches and subsequent cultivation of different cells as well as an initial differentiation of induced pluripotent stem cells into hepatoblast bodies is reported.

The authors thank the German Research Foundation (RTG 2900 nanomaterials@biomembranes, project number 501879556) for funding.

[1]Lancaster, M. A.; Knoblich, J. A. Science 2014, 345, 6194.
[2]Park, S. E.; Georgescu, A.; Huh, D. Science 2019, 364, 6444.
[3]Wang, Y.; He, C.; Xing, W.; Li, F.; Tong, L.; Chen, Z.; Liao, X.; Steinhart, M. Adv. Mater. 2010, 22, 2068.

CBF - D4 - P10
Proteomics in the multi-omics era: A key to safer drugs and deeper disease insights

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Proteomics plays a pivotal role within the broader omics framework by bridging genetic and transcript-level information with functional outcomes at the level of proteins. Since proteins act as the main drivers of cellular activity, proteomic analyses offer insights into biological processes and drug-induced effects that cannot be completely resolved through genomics or transcriptomics alone. When combined with other omics layers such as transcriptomics and metabolomics, proteomics contributes to a comprehensive, system-wide understanding of biological responses relevant to disease and pharmacological interventions.
In this presentation, we emphasize the importance of mass spectrometry-based proteomics as a foundational component of multi-omics approaches in biomedical research and drug safety evaluation. Proteomics enhances these integrative strategies by enabling detailed characterization of protein expression changes, post-translational modifications, and molecular alterations resulting from chemical or pharmaceutical exposure.
To illustrate the breadth of this approach, we present selected case studies demonstrating its application across different research contexts. These include investigations of drug-related protein modifications associated with fluorinated compounds, studies of protein expression changes linked to disease states, and analyses of inflammatory signaling pathways in skin disorders such as psoriasis. Collectively, these examples demonstrate how proteomics can provide mechanistic insights into both therapeutic actions and adverse drug effects.
By establishing proteomics as a central component of integrated omics workflows, this work highlights its essential role in advancing modern pharmacology and translational science. The integration of diverse omics datasets improves mechanistic understanding, facilitates biomarker identification, and strengthens the predictive accuracy of safety assessments. Ongoing developments in analytical methodologies and data integration are expected to further expand the impact of multi-omics strategies in the design of safer and more effective therapeutic solutions.

CBF - D4 - P11
PATHFOOD: From soil to health - Analytical chemistry driving selenium-enriched functional foods

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University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Poland

The development of functional foods enriched with essential micronutrients represents a key challenge at the interface of chemistry, biology, and food science. Selenium (Se), an essential trace element with well-documented health benefits, plays a crucial role in human metabolism, yet its dietary intake remains insufficient in many regions. The PATHFOOD project, coordinated by the University of Warsaw, addresses this issue through an integrated approach combining analytical chemistry, plant science, and food technology.
This study focuses on the design of a sustainable selenium-enriched functional food chain, from biofortification of crops to final product development. Innovative cultivation strategies are applied to enhance selenium uptake in plants while minimizing environmental impact. Subsequent processing methods are optimized to preserve selenium content and bioavailability.
A central aspect of the project is the application of advanced analytical techniques, including inductively coupled plasma mass spectrometry (ICP-MS), for precise quantification and speciation analysis of selenium in plant matrices and food products. These methods enable the assessment of selenium distribution, bioavailability, and safety, ensuring compliance with regulatory standards.
The results demonstrate that combining biofortification strategies with state-of-the-art analytical tools allows for effective monitoring and control of selenium throughout the food production chain. This integrated approach supports the development of safe, high-quality functional foods and contributes to improved public health outcomes.
The PATHFOOD initiative exemplifies how analytical chemistry can bridge the gap between biological systems and food science, fostering sustainable innovation through international collaboration and knowledge exchange.

Funding: This research was funded by the European Union under the Horizon Europe research and innovation programme (2021–2027), within the PATHFOOD project (Creating a Functional and Sustainable Food Chain: A Path to Climate Neutrality and Improved Health in the EU), grant agreement No. 101160011.

CBF - D4 - P12
Identification of isothiocyanate-hydrolyase candidate proteins by in-silico modelling

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Glucosinolate-derived isothiocyanates (ITC) are well known for their health promoting properties, such as anticarcinogenic effects.[1] While ITC also serve as key plant defense compounds, a recent study by Andernach et al.[2] suggested the presence of a plant-endogenous ITC hydrolase (ITCase) in Brassica oleracea. ITCase-mediated breakdown of ITC to amines can result in the loss of these beneficial compounds and to the accumulation of amines whose bioactive properties remain poorly characterized. As the responsible enzyme is not yet identified, this study aims to identify possible candidate proteins by in silico modelling using Boltz-2[3], [4] after protein isolation for further verification as recombinant proteins.
Proteins were extracted from lyophilized Brussels sprouts by sonication after two wash outs, followed by ammonium sulfate precipitation and preparative size-exclusion FPLC. ITCase activity was determined by incubating samples with 3-butenyl ITC and quantifying the resulting amine by LC-MS/MS MRM.[2] Active fractions were analyzed by bottom-up proteomics via nanoLC-HRMS and additionally field asymmetric ion mobility spectrometry (FAIMS) was used due to detergent-induced signal suppression. Annotated proteins with a minimum coverage of 10% and two unique peptides were used for co-folding with 3-butenyl ITC and water as substrates and Zn2+ as a cofactor using Boltz-2.[3], [4]
Of four fractions isolated by preparative size-exclusion FPLC, only for peak 2, which showed the highest absorbance at 280 nm, an ITCase activity of 15% relative to the crude extract was determined, with a purification factor of 5.5. 86 proteins were annotated by bottom-up proteomics by combining nanoLC-HRMS and FAIMS. To further narrow down possible ITCase candidates, in-silico modelling was performed for the annotated proteins. For 14 out of 86 proteins the predicted 3D structures contained promising active centers consisting of Zn2+ coordinated mainly by histidine residues and the substrates located near the metal ion, while achieving acceptable to good quality parameters. These 14 candidate proteins represent potential plant-endogenous ITCases in B. oleracea and will be prioritized for recombinant expression and functional validation.

[1]D. L. Palliyaguru et al.; Mol. Nutr. & Food Res.; 2018, 62, 1700965; doi.org/10.1002/mnfr.201700965
[2]L. Andernach et al.; Food Chemistry; 2023, 405, 134907; doi.org/10.1016/j.foodchem.2022.134907.
[3]Rowan Scientific. https://www.rowansci.com (accessed 2026-03-26).
[4]S. Passaro et al.; bioRxiv; 2025, doi.org/10.1101/2025.06.14.659707.

CBF - D4 - P13

Click! Bioconjugate! Release!: A unified diazaborine platform for stimuli-responsive therapeutics

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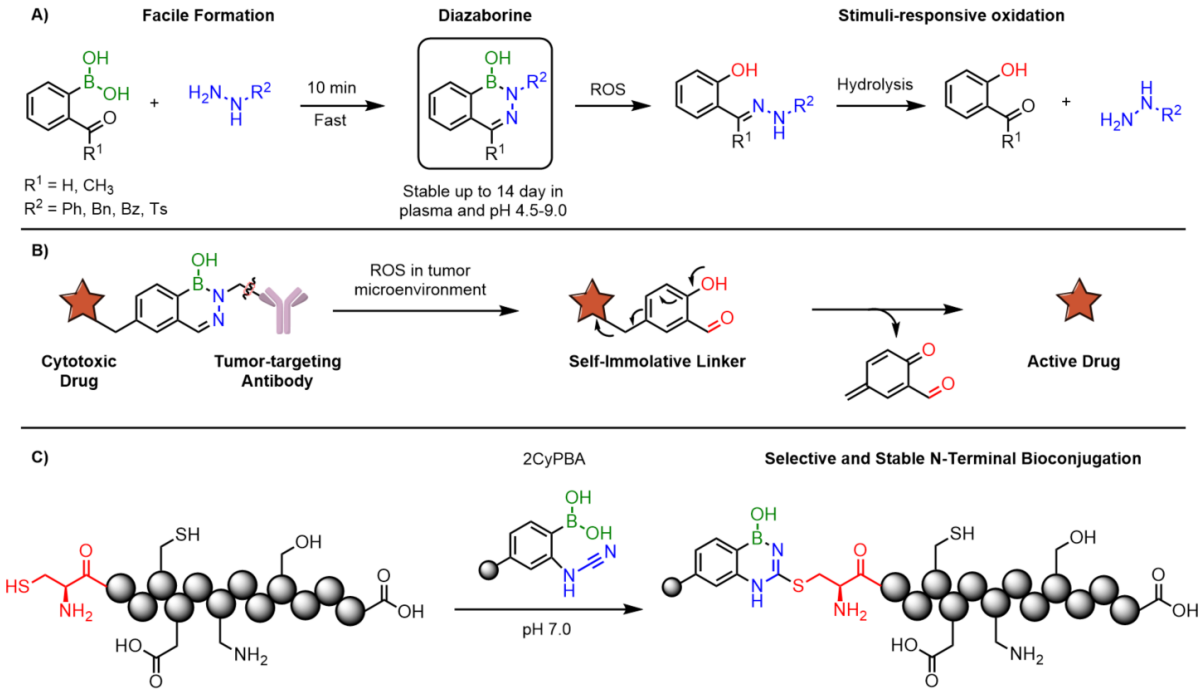
Antibody-drug conjugates (ADCs) are among the most promising therapeutic strategies in oncology. Central to their success is the linker, since it must remain stable in circulation but release the payload selectively within cancer cells. We recently developed diazaborines (DABs) as a novel ROS-responsive motif, exploiting the oxidative microenvironment of tumors to enable the design of a first-in-class ROS-activatable ADC. DABs form rapidly under bioorthogonal conditions (pH 7.4, 10 min), display excellent stability in buffer and plasma (pH 4.5–9.0), and are readily oxidized by H_2O_2 ($t_1/_2$ = 15 min with 100 equiv.). A DAB-based self-immolative linker was incorporated into a homogeneous ADC bearing SN-38 and a B-cell lymphoma-targeting antibody, yielding potent activity (IC_{50} = 54.1 nM) and high selectivity (>100 μM in T-cell lymphoma). To expand the utility of this chemistry, we developed a site-selective strategy for installing DABs directly onto peptides via chemoselective cysteine alkylation. Using (2-cyanamidophenyl)boronic acids (2CyPBAs), DABs can be formed *in situ* through selective reaction with *N*-terminal cysteines, guided by an intramolecular B–N bond. The reaction proceeds under mild, aqueous conditions, shows high conversion across diverse peptide sequences, and exhibits strict selectivity over internal cysteines. This method gives new life to DAB chemistry by enabling its direct incorporation without the need for auxiliary bioconjugation handles and opening new opportunities for targeted therapeutics and functional bioconjugates.



Acknowledgements: We thank the FCT for financial support (2022.06817.CEECIND and 2024.16254.PEX)

[1] J. P. M. António et al, Chem. Soc. Rev. 2019, 48, 3513.
[2] J. P. M. António et al, Angew. Chem. Int. Ed. 2021, 60, 25914
[3] J. P. M. António et al, Org. Lett. 2023, 25, 5476–5480.

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Catalyzing New Chemistry Solutions (CCS)

CCS - D4 - P04

Modification of Ni/Al_2O_3 catalysts by incorporating graphitic Carbon Quantum Dots (CQDs) for selective CO_2 hydrogenation to CO

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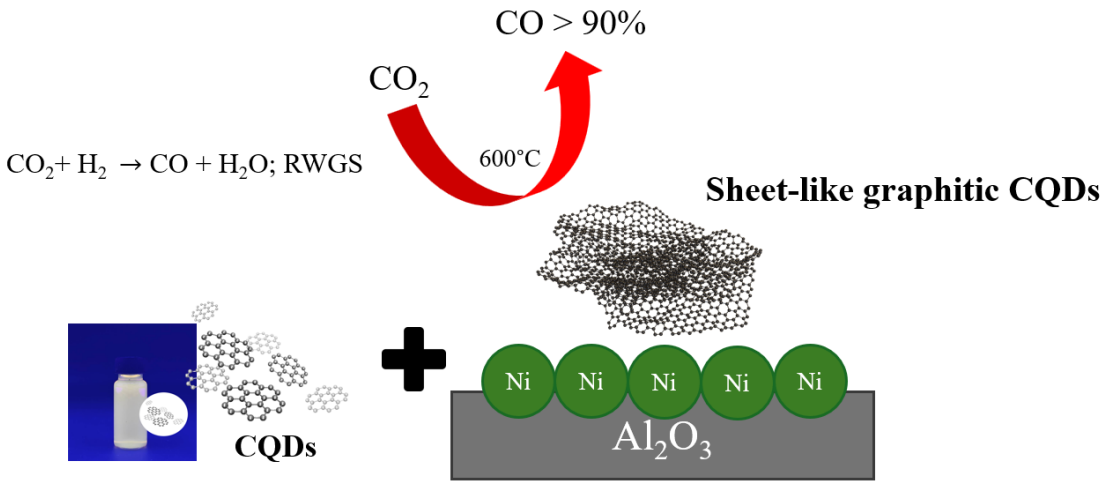
CO_2 emissions are a major driver of global warming and climate change. One promising mitigation strategy is the hydrogenation of CO_2 into fuels and chemicals. However, despite CO being a crucial intermediate for producing higher-value liquid hydrocarbons and oxygenates, achieving high CO selectivity over Ni catalysts remains challenging. In this study, 15 wt.% Ni/Al_2O_3 catalysts (15Ni) were modified with 3 wt.% graphitic carbon quantum dots (CQDs) via incipient impregnation and calcination under N_2 at 600 °C for 5 h. The structural and surface properties were characterized by SEM-EDX, TEM-EDX, ETEM, XRD, XPS, ICP, TGA, TPO-MS and H_2-TPR-MS analyses.

While the convetional 15Ni catalyst mainly yielded methane and formed soft coke after 10 h at 600°C, the incorporation of CQDs markedly enhanced CO selectivity. The 15Ni3CQD catalyst achieved ~90% CO selectivity with ~57% CO_2 conversion, with no evidence of soft coke formation. Moreover, CQDs underwent in situ transformation into sheet-like graphitic carbon layers on the catalyst surface, contributing additional value. These findings demonstrate that CQDs promote the reverse water–gas shift (RWGS) pathway while suppressing methanation, thereby steering Ni-based catalysts toward CO production. Overall, this work highlights CQDs as an effective, scalable, and non-noble modifier for CO_2 hydrogenation, offering a promising route for sustainable CO_2 utilization.

Graphical abstract:



CCS - D4 - P07
Sustainable synthesis of 2,4,6-trisubstituted pyridines using surface-modified PET@UiO-66 vials

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National Institute of Technology Warangal, India

This study demonstrates the modification of a polyethylene terephthalate (PET) surface to fabricate a metal-organic framework (MOF)-based UiO-66 vial for application in multicomponent reactions.[1] We report the development of a PET@UiO-66 vial that functions as an efficient, robust, and reusable heterogeneous catalyst for the sustainable synthesis of 2,4,6-trisubstituted pyridines via a multicomponent reaction strategy.[2] The structural and morphological features of the fabricated PET@UiO-66 vial were systematically characterized using powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR), optical microscopy, and field-emission scanning electron microscopy (FESEM). Nitrogen adsorption-desorption isotherm analysis revealed a specific surface area of 564.36 m^2g^{-1}, a maximum pore volume of 0.06 cm^3g^{-1}, and an average pore diameter of 3.05 nm.[3] Optimization of the reaction parameters indicated that the use of tert-butyl hydroperoxide (TBHP) as an oxidant in tetrahydrofuran (THF) at 60 °C afforded good to excellent yields of the desired products. The key advantages of this methodology include the high stability of the surface-modified vials, excellent recyclability, and operational simplicity, making it a sustainable and practical approach for heterocycle synthesis.

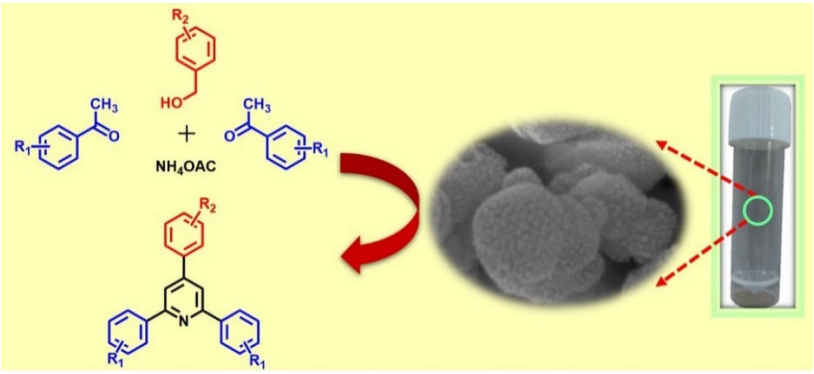

Fig. 1. Fabrication of a reusable PET@UiO-66 vessel for sustainable multicomponent synthesis of trisubstituted pyridines.

We greatly acknowledge the financial support from the SERB (sanction order no: CRG/2023/002466) and DST FIST (SR/FST/CS-II/2018/65). The authors gratefully acknowledge the University Grants Commission (UGC) for the research fellowship and the National Institute of Technology Warangal for providing infrastructural support.

[1]Shaabani, A.; Mohammadian, R.; Hooshmand, S. E.; Hashemzadeh, A.; Amini, M. M., *ChemistrySelect* **2017**, *2*, 11906–11911.
[2]Rohokale, R. S.; Koenig, B.; Dhavale, D. D.. *J.*, *Org. Chem.* **2016**, *81*, 7121–7126.
[3]Winarta, J.; Shan, B.; McIntyre, S. M.; Ye, L.; Wang, C.; Liu, J.; Mu, B., *Cryst. Growth Des.* **2020**, *20*, 1347–1362.

CCS - D4 - P18

Bubbles templated porous CeSe2/Co3Se4 heterostructures supported on Ni foam for CO2-free selective methanol oxidation to enhance green hydrogen production

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This study investigates methanol-assisted water splitting (MAWS) as a promising alternative to conventional water electrolysis, with a focus on developing novel electrocatalysts to enhance the efficiency and selectivity of the methanol oxidation reaction (MOR) and the hydrogen evolution reaction (HER). A three-step synthesis process (electrodeposition, annealing, and selenization) was employed to synthesize the bubble-templated porous CeSe2/Co3Se4 heterostructures supported on nickel foam (CeCoSe@NF). The electrocatalyst's activity and selectivity for MOR to formate were tested, and its performance was evaluated by Operando electrochemical impedance spectroscopy (EIS) and H-NMR. The optimized electrocatalyst required a potential less than 1.35 V vs. RHE to initiate the methanol oxidation reaction, achieving a current density of 100 mA cm−2 at just 1.44 V vs. RHE under alkaline conditions. Operando EIS further confirms that MOR begins at 1.3 V for the porous CeCoSe@NF electrocatalyst, and MOR occurs similarly to OER at the low-frequency interface, indicating that MOR activity comes from the same adsorption intermediate (OH*) as OER. For overall methanol-assisted water electrolysis, the optimized porous heterostructured CeO2/Co3O4@NF electrode (CeCo@NF) without selenization showed good performance for HER, requiring 170 mV overpotential to attain 100 mA cm-2 current density with near 98 % Faradaic efficiency. The two-electrode integrated electrolyzer (CeCoSe@NF as the anode and CeCo@NF as the cathode), with methanol-assisted splitting, operates at a cell voltage of only 1.52 V to reach 20 mA cm-2, which is significantly lower than the 1.65 V required for traditional water splitting under the same conditions. The superior performance is attributed to the porous, dendritically interconnected nanostructure, synergistic heterointerfaces, and strong electronic coupling between the active components and the conductive Ni foam. This study highlights the potential of targeted methanol oxidation as a dual-purpose strategy for efficient energy-saving hydrogen generation and methanol upgrading to formate, contributing to the development of more sustainable energy systems.

CCS - D4 - P22

4,4'-oxybis-benzoic acid-based pristine MOFs as reusable, heterogeneous catalyst for hydrogenation reactions

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The large surface area, adjustable pore environment, and modular structural design of Metal-Organic Frameworks (MOFs) make MOFs a flexible class of porous crystalline materials with enormous potential in heterogeneous catalysis. The development of transition metal-based MOF catalytic systems for industrially significant organic transformations is the main goal of this effort; major focus on hydrogenation reactions, dehalogenation processes, and carbon–carbon and carbon–heteroatom coupling reactions. To modify active sites, electrical characteristics, and catalytic accessibility, several mono-metallic, bi-metallic, and bi-linker MOFs are created by carefully choosing metal nodes and organic linkers[1]. The integration of several 3d transition metals and mixed linkers is investigated to provide synergistic effects, improve catalytic efficiency, and expand substrate scope. The 3d transition metals such as Ni, Mn, Zn, and Cu-based MOFs are synthesized *via* the traditional solvothermal method using the organic linker 4,4'-oxybis-benzoic acid (OBA), which is a pristine linker with much enhanced coordination towards metals for the framework development. The structural integrity and characteristics of the produced MOFs are methodically assessed using spectroscopic techniques[2]. These MOFs demonstrate effective catalytic activity, selectivity, and recyclability under mild and sustained reaction conditions. This study also focuses on synthesizing a novel MOF using the OBA ligand coordination to the aluminium metal center to form stable 3-D framework systems to catalyze the major organic reactions. Understanding structure–activity correlations, metal–ligand collaboration, and the function of framework porosity in promoting reactant diffusion and product formation are all given consideration. The findings demonstrate the efficacy of tailored MOF structures as reliable and reusable heterogeneous catalysts for organic transformations that are significant to industry and the environment.

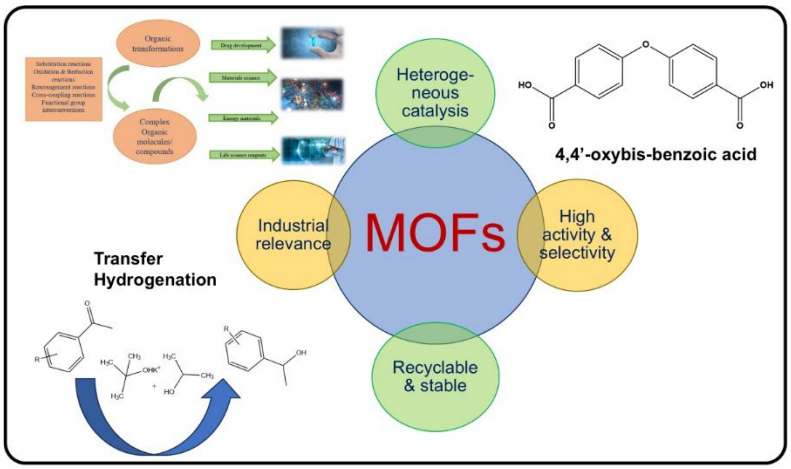

Fig. 1. MOF-based Catalytic systems for industrially important organic reactions

[1]Dhakshinamoorthy, A., Asiri, A. M., & Garcia, H. Chem. Soc. Rev., **2015**, 44,1922.
[2]Dhayanithi, C. A., & Babu, S. G. Microchimica Acta, **2024**, 191(10), 611.

CCS - D4 - P25
Dehydrogenation of methanol to methyl formate using $CuO/CuAl_2O_4/Al_2O_3$-catalysts

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The dehydrogenation of methanol to methyl formate is a promising alternative to the carbonylation of methanol with carbon monoxide. Mostly Cu-bearing catalysts are used for the dehydrogenation of methanol, yielding 22 – 36 % of methyl formate in a temperature range of 200 – 310 °C.[1] We investigated 3 different catalyst compositions (40, 50 and 60 mol% CuO with 60, 50 and 40 mol% Al_2O_3 respectively) at three different calcination temperatures (800, 950 and 1100°C), which led to nine different catalysts comprised of CuO, $CuAl_2O_4$, $CuAlO_2$ and Al_2O_3. The catalysts were prepared by coprecipitation of copper and aluminium citrate. The $CuO/CuAl_2O_4/Al_2O_3$-catalysts were tested for the methanol dehydrogenation at 210, 240 and 270 °C without prior reduction. CuO undergoes rapid reduction to Cu^0 under the reaction conditions while $CuAl_2O_4$ slowly releases Cu^0 and Al_2O_3. The highest methyl formate yield of 30 % is achieved at 270 °C with a catalyst composition of 60 mol% CuO and 40 mol% Al_2O_3 and a calcination temperature of 800 °C. If the calcination temperature increases to 950 °C, the yield decreases to 25 % but the methyl formate selectivity rises from 51 to 89 %. The methyl formate yield increases to 35 - 40 % after 15 h of reaction time because the conversion increases due to the slow reduction of $CuAl_2O_4$. After 24 h the yield decreases to 30 % due to selectivity increases for dimethyl ether and carbon monoxide. This equals 83 % of the equilibrium methyl formate yield of 36 % at 240 °C reaction temperature.

[1]Li, Y.; Zhao, J.; Yan, A.; Quan. Y.; Ren. J. *Fuel* **2025**, *388*, 134520.

The 10th EuChemS Chemistry Congress

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Energy, Environment & Sustainability (EES)

EES - D4 - P01
Treatment of poly(vinyl chloride) and study of its pyrolysis outcomes

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University College Dublin, Ireland

Pyrolysis is a chemical recycling method used for plastic waste management, which involves heating plastic waste to temperatures of 300-800˚C in the absence of oxygen to generate useful condensable and non-condensable products.
Poly(vinyl chloride) (PVC) is the third most widely produced plastic in the world, however progress in the pyrolysis of PVC has been hindered by the fact that it contains chlorine. The HCl generated from pyrolysis causes corrosion, slag formation, and the generation of toxic organochlorines.[1] In this work, the optimal conditions for PVC pyrolysis were determined using thermogravimetric analysis.
To combat the issues with chlorine and HCl in waste PVC, different PVC pre-treatment strategies for chlorine removal were studied. Thermal dechlorination was performed by low temperature pyrolysis in a thermogravimetric analyser. Solvothermal and non-thermal plasma treatments, which introduce oxygen species that partake in elimination and substitution reactions, were also investigated. The outcomes from PVC treated in these ways were compared with those from virgin PVC using thermogravimetric analysis and within a lab-scale pyrolysis reactor.
Heterogenous aluminosilicate catalysts have been shown to increase the rate of plastic degradation during pyrolysis, facilitating complete degradation at lower temperatures than in the absence of a catalyst.[2] The effects of aluminosilicate solid catalysts on the degradation of virgin and treated PVC were studied.

This project has received funding from the European Union HORIZON TMA MSCA Staff Exchanges (HORIZON-MSCA-2021-SE-01), grant agreement no. 101086071, project name “CUPOLA — Carbon-neutral pathways of recycling marine plastic waste”.

[1] Tian, Y.; Han, M.; Gu, D.; Bi, Z.; Gu, N.; Hu, T.; Li, G.; Zhang, N.; Lu, J. PVC Dechlorination for Facilitating Plastic Chemical Recycling: A Systematic Literature Review of Technical Advances, Modeling and Assessment. *Sustainability* **2024**, *16* (19), 8331.
[2] Papuga, S.; Djurdjevic, M.; Ciccioli, A.; Vecchio Ciprioti, S. Catalytic Pyrolysis of Plastic Waste and Molecular Symmetry Effects: A Review. *Symmetry* **2023**, *15* (1), 38.

EES - D4 - P02

High performance steam methane reforming via tuned metal support interactions in NiMg-Yb_2O_3 sesquioxide: Activity, stability, and coke resistance

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Recently, high-performance and coke-resistant catalysts are essential to produce hydrogen via steam methane reforming (SMR) at lower operating temperatures. In present work, NiMg-Yb_2O_3 catalyst with selective interactions between metals on the support is achieved through a controlled coprecipitation approach using ethylene glycol as a structure-directing medium, which produced a unique cauliflower-like morphology with high surface energy nanoparticles. The addition of Mg and Ni in Yb_2O_3 was effective in altering the physicochemical characteristics of the Yb_2O_3 base which promoted the dispersal of metals and the strength of interactions between metals and the support. The catalyst shows an excellent SMR activity with an excellent methane conversion of 97% and hydrogen production value of 92.75% at a low operating temperature of 650 °C. Cauliflower-like morphology enabled the enhanced diffusion of the reactants and exposure of the active sites, which led to high catalytic activity. Moreover, co-interaction of Ni, Mg and Yb_2O_3 greatly inhibited carbon deposition resulting in high stability and coke resistance in a long-term reaction time. These findings indicate that the resultant material fabricated via ethylene glycol-assisted coprecipitation of NiMg-Yb_2O_3 can attain morphology control to form effective low-temperature, high-efficiency SMR catalysts for hydrogen production.

EES - D4 - P03
Phase stability and thermodynamic properties of magnesium carbonates in salt solutions

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The long-term safety assessment of radioactive waste repositories is largely based on thermodynamic modelling, which requires a robust understanding of chemical equilibria between host rock components, saline pore fluids, waste inventories, and engineered barrier materials. In particular, carbonate concentration and pH significantly impact the actinide solubility. In current rock-salt-based repository concepts, these parameters are planned to be actively controlled by the addition of MgO or $Mg(OH)_2$ respectively, which bind CO_2, ensure an alkaline pH of brines, and promote carbonate formation. So far however, the stability and transformation behavior of magnesium carbonate phases under repository-relevant ionic strengths remain insufficiently understood.
Current studies are thus focused on the exploration of any chemical equilibria involved in the system Mg^{2+}–Cl^-–OH^-–CO_2–H_2O, aiming to expand the Thermodynamic Reference Database (THEREDA).[1,2] The solid magnesium carbonate phases magnesite ($MgCO_3$), nesquehonite ($MgCO_3 \cdot 3\ H_2O$), hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4\ H_2O$), dypingite ($Mg_5(CO_3)_4(OH)_2 \cdot 5+x\ H_2O$), and chlorartinite ($Mg_2(CO_3)Cl(OH) \cdot x\ H_2O$) have been deemed most relevant, and syntheses have been established that reproducibly lead to well-defined solids as characterizations using P-XRD, SEM (e.g. Fig. 1), Raman, and TG-DSC have shown. The presented experimental setups designed to quickly establish equilibria with $MgCl_2$ solutions of differing concentrations at a given temperature and subsequently allowing for quantifying the composition of both liquid and gas phases are essential to accurately and fully describe the system. A crucial aspect is determining the speciation of ions present, as well as their interactions in solution according to the PITZER model. As very low concentrations ($b < 10^{-5}$ mol kgw^{-1}) of CO_3^{2-} and OH^- complexes are expected, specifically tailored analytical methods need to be explored.

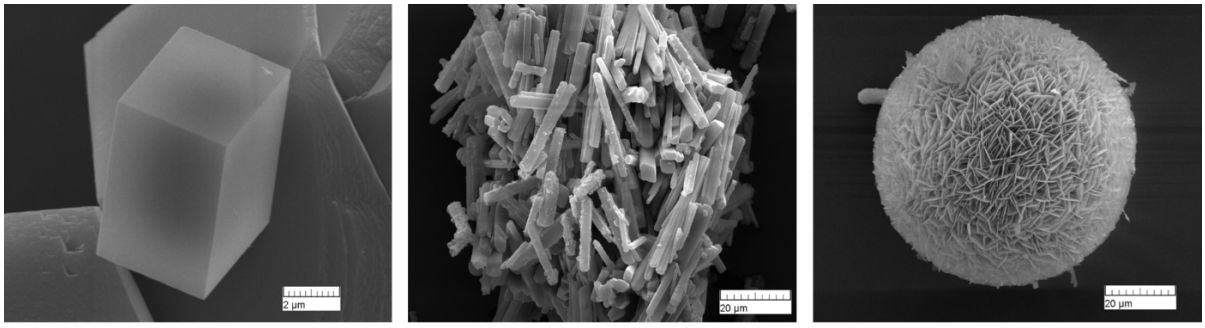

Fig. 1. SEM images of prepared solids; magnesite, nesquehonite, and hydromagnesite.

[1]Moog, H. C.; Bok, F.; Marquardt, C. M.; Brendler, V. *Appl. Geochem.* **2015**, *55*, 72–84.
[2]Moog, H. C.; Altmaier, M.; Bok, F.; Brendler, V.; Freyer, D.; Gaona, X.; Hagemann, S.; Joseph, C.; Miron, G.-D.; Pannach, M.; et al. *Appl. Geochem.* **2026**, *196*, 106646.

EES - D4 - P04

Removal of metallic fragments contained in the waste generated during the manufacturing of photovoltaic cells

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The photovoltaic panel industry generates a significant amount of slurry during the wafering stage, which involves two main techniques: slurry wire sawing and diamond wire sawing. This process produces effluents rich in pure silicon particles (up to 40%), silicon carbide (SiC), iron (Fe), and polyethylene glycol (PEG). In order to reduce costs and optimize the production of photovoltaic cells, it is crucial to recover and treat this waste.
The effluent was collected and analyzed by FTIR-ATR spectroscopy, highlighting the chemical composition of the PEG lubricant, which was purified for potential reuse. A physicochemical treatment protocol was implemented to separate the liquid and solid phases, with optimization of the washing conditions. The solid phase was characterized by FTIR-ATR and XRD, while the liquid phase underwent thermogravimetric analysis (TGA).
The study of metallic fragments present in the waste was carried out using electron probe microanalysis (EPMA), and dry magnetic separation was explored to remove these fragments. The results allowed for an evaluation of the effectiveness of this separation technique. Finally, the efficiency of this separation technique was assessed by EDX analysis of the magnetic and non-magnetic phases, enabling the identification of the elements present in each phase.

Keywords: Slurry; PEG; Photovoltaic; Metallic fragments; Characterization.

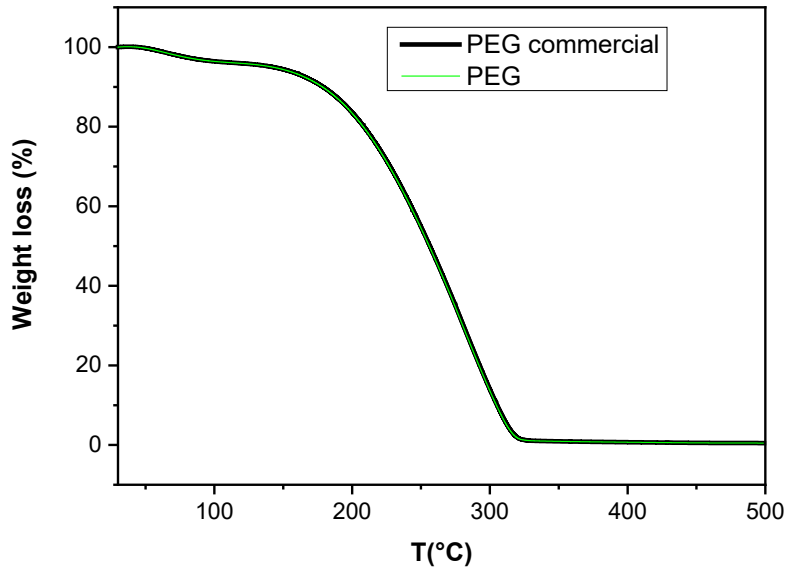

Fig. Thermograms (TGA/DTG) of regenerated PEG and commercial PEG.

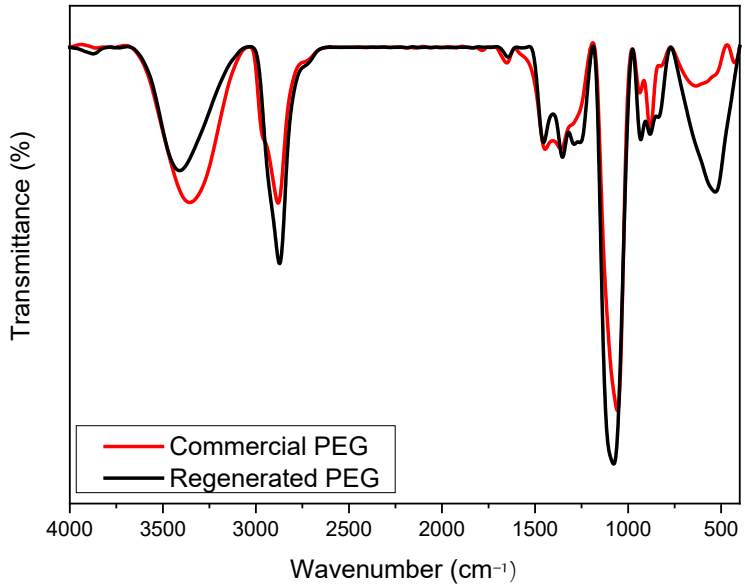

Fig. FTIR-ATR spectra of the liquid phase of regenerated PEG and commercial PEG.

The efficiency of the lubricant was evaluated by characterizing both the regenerated lubricant and the commercial lubricant used as a reference, using FTIR and thermogravimetric analysis (TGA).
The FTIR-ATR spectra of commercial PEG and regenerated PEG were compared. Both spectra exhibit a general similarity, except in the region between 3200 and 3400 cm^{-1}.
In the spectrum of commercial PEG, an intense band is observed in this region, which is likely attributed to the O–H stretching vibration. In contrast, the spectrum of regenerated PEG shows a less intense band, which may correspond to a combination of O–H vibrational modes.

EES - D4 - P05

Identifying complexing agents for the selective binding of Pb^{2+} released during perovskite solar cell degradation

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[1]Swansea University, UK; [2]University of KwaZulu-Natal, South Africa

Perovskite solar cells (PSCs) are an exciting, emerging photovoltaic technology showing promise for circular economy applications and contributing to net-zero targets. Currently, PSCs demonstrate power conversion efficiencies up to 27.3 %, aided by a high absorption coefficient and ideal bandgap. However, exposure to moisture, oxygen, heat or light decomposes the Pb-containing perovskite layer into water-soluble lead salts, Pb^{2+}. These species may leach into the environment when modules are damaged during use or end-of-life processing. This leads to harmful accumulation in our biosphere, ultimately impacting human health. To mitigate this, colourimetric methods were explored to assess dyes that selectively bind Pb^{2+}, enabling early detection of PSC degradation and prevention of lead release. Metal–ligand interactions were observed using UV–Vis absorbance alongside visual colour observations to evaluate binding behaviour and complex strength. By binding Pb^{2+} as it forms, these dyes support sequestration while simultaneously offering a visual indication of degradation, creating an approach that reduces environmental emissions and supports real-time monitoring of PSC stability.

[1] Charles, R. G.; Doolin, A.; Rodriguez, R. G.; Villalobos, K. V.; Davies, M. L. Energy Environ. Sci. 2023, 16, 3711–3733.
[2] National Renewable Energy Laboratory (NREL). Best Research-Cell Efficiency Chart. https://www.nrel.gov/pv/cell-efficiency (accessed Feb 2025).
[3] Chen, J.; Park, N.-G. ACS Energy Lett. 2020, 5, 2742.
[4] Ren, M.; Qian, X.; Chen, Y.; Wang, T.; Zhao, Y. J. Hazard. Mater. 2022, 426, 127848.
[5] Su, P.; Liu, Y.; Zhang, J.; Chen, C.; Yang, B.; Zhang, C.; Zhao, X. J. Phys. Chem. Lett. 2020, 11, 28129
[6] Luo, H.; Li, P.; Ma, J.; Han, L.; Zhang, Y.; Song, Y. Adv. Energy Mater. 2022, 12, 2201242.

EES - D4 - P06
Comparison of hydrogel coated ion selective solid-state electrodes for nitrate measurements in soil

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[1]*University of Connecticut, USA*

Understanding temporal dynamics of nitrate in agricultural soils during different management strategies would help reduce nitrogen leaching to the downstream environment. However, the best methods to examine that are extraction techniques, while *in-situ* measurements are difficult due to variations in moisture content in soils leading to loss of sensor contact with porewater. In order to address this limitation, three hydrogel coatings, acrylamide, lignin and agar, were applied to an established ion selective solid-state electrode for nitrate and compared in terms of linearity of response, range of measurement, and response time for stabilization. All hydrogel options gave reasonable calibrations with Nernst slopes within 20% of ideal in aqueous solution over an extended concentration range of 0-100 mg L NO_3^-N, relevant to agricultural soils. Calibrations in soil mixtures indicated minimal adsorption and loss of nitrate, but the lignin hydrogel resulted in a significant delay in response and reduction in calibration quality, whereas the agar maintained a similar response to aqueous calibration steps (Figure 1). A test was conducted to assess the rate of nitrate diffusion through the hydrogels and time to stabilization and found that the nitrate concentration across the acrylamide did not stabilize within 6 hours, lignin took 4 hours, and agar stabilized within 1 hour. The agar coated ion selective electrode was applied in a moisture controlled soil environment and maintained a valid nitrate reading over the course of a few days in soil at field capacity, but deviated from the measured porewater concentration as soil moisture decreased substantially. Further adjustments to the calibration as a function of soil moisture would help in estimating porewater nitrate concentrations in actual soils.

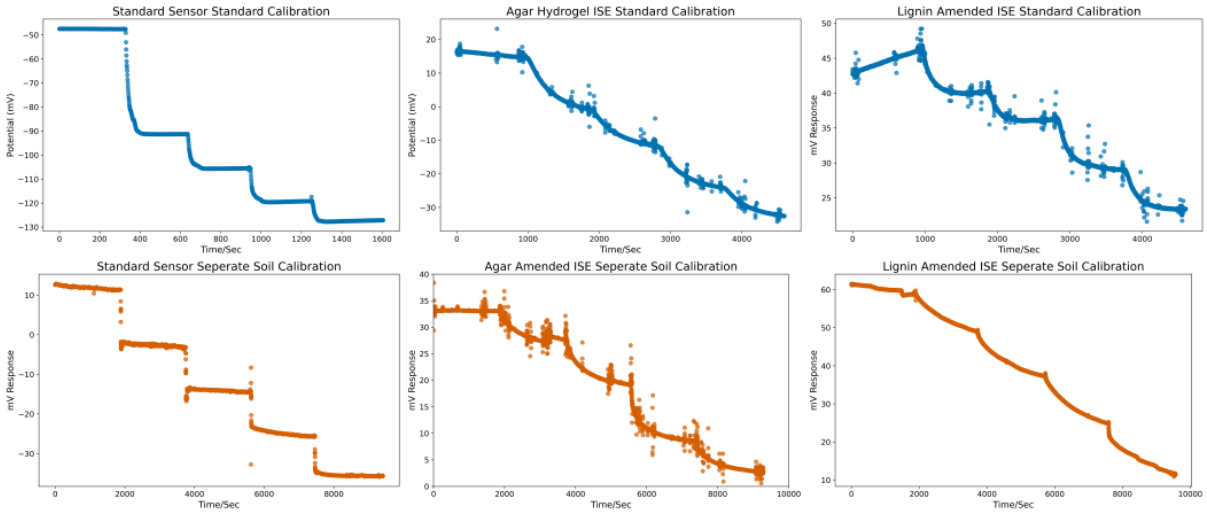

Fig. 1. Calibration comparison of uncoated, agar, and lignin coated ion selective electrodes in solution and soil mixtures.

EES - D4 - P07

Monoatomic copper-anchored UiO-66-NH_2 as a mechanistically defined Lewis acid catalyst for CO_2 cycloaddition and enantioselective Strecker synthesis

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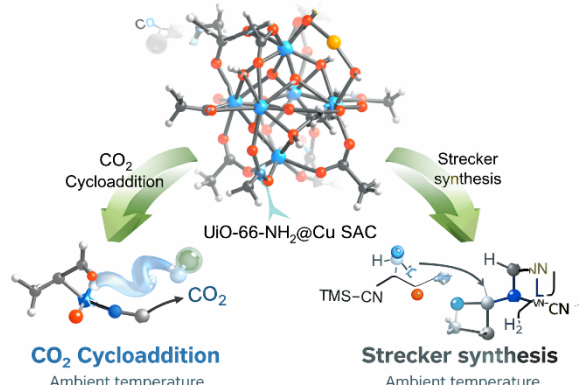
[1]Czech Advanced Technology and Research Institute (CATRIN), Regional Centre of Advanced Technologies and Materials (RCPTM), Palacký University Olomouc, Czech Republic

Single-atom catalysts (SACs) have emerged as an advanced class of heterogeneous catalysts due to their maximal atom efficiency and well-defined active sites; however, stabilizing isolated metal atoms while controlling their coordination environment remains a significant challenge [1,2]. In this work, we report a monoatomic copper-anchored metal–organic framework (UiO-66-NH_2@Cu SAC) as a robust Lewis acid catalyst for CO_2 cycloaddition to epoxides and enantioselective Strecker synthesis of α-aminonitriles.
The amine-functionalized UiO-66-NH_2 framework provides strong Cu–N coordination sites that immobilize isolated Cu(II) atoms within the Zr_6-based lattice, generating electronically unsaturated and spatially isolated Lewis acidic centers [3]. In CO_2 cycloaddition, the single Cu site activates epoxides via Lewis acid coordination to the oxygen atom. At the same time, the confined-pore environment facilitates CO_2 insertion and suppresses competing side reactions, thereby achieving high selectivity toward cyclic carbonates [4]. In the Strecker reaction, cooperative activation of imine substrates by isolated Cu Lewis acid sites, combined with steric confinement within the MOF pores, enables efficient stereochemical control, affording α-aminonitriles with high enantiomeric excess. The atomically dispersed Cu sites effectively prevent aggregation and leaching, resulting in excellent catalytic stability and recyclability without loss of activity or enantioselectivity. This study highlights how coordination-defined single Cu sites and confinement effects govern reactivity and selectivity, demonstrating UiO-66-NH_2@Cu SACs as a versatile platform for sustainable CO_2 valorization and asymmetric synthesis.



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[1]Qiao, B.; et al. *Nat. Chem.* **2011**, *3*, 634–641.
[2]Liu, L.; Corma, A. *Chem. Rev.* **2018**, *118*, 4981–5079.
[3]Li, Z.; et al. *J. Am. Chem. Soc.* **2020**, *142*, 17671–17679.
[4]Aresta, M.; Dibenedetto, A. *Chem. Rev.* **2007**, *107*, 428–452.

EES - D4- P08
Scale-up, shaping, and catalytic performance of MIL-100(Fe) in propane oxidation

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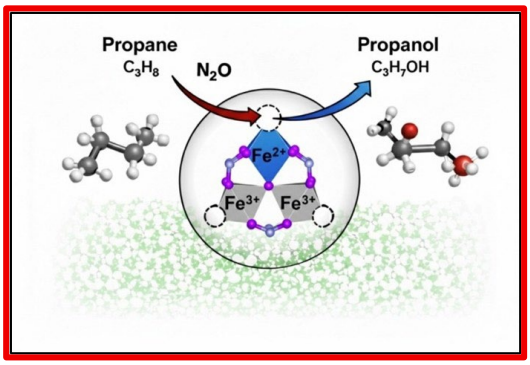
[1]Dept. of Chemistry, NIS and INSTM Reference centre University of Turin, Italy; [2] Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 – UCCS - Unite´ de Catalyse et Chimie du Solide, France; [3]Johnson Matthey Technology Centre, UK

Iron-based metal–organic frameworks (MOFs) are promising catalysts for selective oxidation of light alkanes, but their practical application requires scalable synthesis, suitable shaping, and stable catalytic performance[1,2]. In this study, MIL-100(Fe) synthesis was upscaled (140 g batch) and the product was shaped into pellets and binder-containing granules for operation in a fixed-bed reactor. The synthesized material was shaped into pellets and binder-containing granules to allow operation under industrially relevant conditions[1,3,4]. X-ray diffraction confirmed that the crystalline structure was preserved after shaping. BET surface area measurements showed only a moderate decrease due to mechanical compression and binder addition. SEM–EDX analysis revealed uniform morphology and homogeneous elemental distribution, while thermogravimetric analysis demonstrated unchanged thermal stability. In situ FTIR spectroscopy with CO as a probe molecule confirmed the presence of accessible Fe^{3+} and Fe^{2+} redox sites after activation at 250 °C. Catalytic tests for propane oxidation to propanol were carried out in a fixed-bed reactor. All shaped samples showed stable propanol production with no significant differences in steady-state productivity. These results demonstrate that MIL-100(Fe) maintains its structural integrity and catalytic performance after shaping and is suitable for selective propane oxidation in fixed-bed reactors.



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[1]Chen, H.; Wang, Q.; Chen, L.; Cai, S.; Lei, J.; Li, S. *Chem and Bio Engineering* **2024**, *1* (10), 817–825.
[2]Groppo, E.; Rojas-Buzo, S.; Bordiga S.; *Chemical Reviews*. American Chemical Society November 8, **2023,** pp 12135–12169.
[3]Castner, A. T.; Johnson, B. A.; Cohen, S. M.; Ott, S.. *J. Am. Chem. Soc.* **2021**, *143* (21), 7991–7999.
[4]Paul, T.; Juma, A.; Alqerem, R.; Karanikolos, G.; Arafat, H. A.; Dumée, L. F.. *Journal of Environmental Chemical Engineering*. Elsevier Ltd October 1**, 2023**.

EES - D4 - P09

Clay-based platforms for REE recovery: Selective adsorption, regeneration and magnetic separation

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Growing technological dependence on rare earth elements (REEs) is driving the search for recovery routes that are both efficient and environmentally responsible. A particularly attractive pathway is adsorption from contaminated waters and leachates produced by industrial operations and mining-related activities, where dilute streams can still represent significant resource value.

This study investigates how naturally abundant clays, notably vermiculite and bentonite, can be progressed from low-cost raw minerals into engineered clay-based nanocomposites for REE capture. We discuss the design logic behind this transition: leveraging clay ion-exchange and surface chemistry, then enhancing performance through functionalisation with spinel ferrite nanoparticles (to enable magnetic separation) and biopolymers (to introduce tailored binding sites), while keeping regeneration and reuse as central requirements. Emphasis is placed on performance in realistic matrices and on practical regeneration strategies.

A central case study focuses on Nd and Dy recovery from end-of-life permanent magnet leachates using expanded vermiculite and vermiculite-derived nanocomposites. Under single-element conditions, raw vermiculite reached sorption capacities of 485 μmol g^{-1} (Nd) and 210 μmol g^{-1} (Dy). In acidic multimetal leachates, uptake followed the sequence Fe > Nd > Zn > Pr > Co > Dy > Ni > Al > Mn, revealing strong competition effects. Although very high total capacities were achieved (up to 12 mmol g^{-1}), selectivity remained limited. For desorption, chelating agents outperformed other eluents, and EDTA showed preferential Nd desorption relative to competing metals, an important result given the difficulty of separating REEs. Post-sorption characterisation indicated that vermiculite largely retained its layered structure, functional groups, chemical composition, and thermal stability.

Overall, clay-based nanocomposites, especially magnetically responsive systems, offer a promising, scalable platform for coupling water remediation with REE recovery, while highlighting that future progress hinges on improving selectivity in complex leachates.

This work was funded by the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) (Grants 2017/18236-1 and 2019/11353-8), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) (Grant 88887.571776 / 2020-00), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) (Grants 406193/2018-5 and 308046/2019-6). This work was also developed within the scope of the project CICECO Aveiro Institute of Materials, UID/50011/2025 (DOI 10.54499/UID/50011/2025) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).Cláudia B. Lopes thanks Fundação para a Ciência e a Tecnologia (FCT) for her researcher contract (CEECIND/03739/2021).

EES - D4 - P10

Activated carbon production from exhaustive olive pomace: Simulation process and autothermal pyrolysis

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The agri-food industry generates large amounts of organic residues whose inadequate management leads to environmental and economic challenges. Exhausted olive pomace (EOP), a by-product obtained after the second extraction of olive oil, is produced in significant quantities in Mediterranean countries and poses particular risks due to its phenolic content, moisture, and high organic load. EOP is an excellent carbon precursor for the production of activated carbon with high uptake capacity [1]. This study investigates the valorization of EOP through its transformation into activated carbon by means of an autothermal pyrolysis process. The objective is to determine whether the system can sustain the thermal energy required for pyrolysis without external heat input under different cases: (1) combusting either a fraction of the raw biomass, (2) part of the resulting biochar, or (3) generated gases. Experimental characterization of real EOP samples was performed using thermogravimetric analysis (TGA) and elemental analysis to determine proximate and ultimate compositions. These results were incorporated into an Aspen Plus V15 simulation framework (Figure 1), where EOP, biochar, and ash were treated as non-conventional components. Results indicate that autothermal operation is feasible in both scenarios; however, combusting biochar is more energy-efficient due to its higher fixed-carbon content and calorific value. Autothermicity is achieved when approximately 43% of the biochar is burned, compared to 14% of the EOP feed. Furthermore, routing the pyrolysis gases to combustion significantly increases net heat production, reaching up to 354 kW versus 36 kW when gases are not recovered. Hydrogen and light hydrocarbons are consistently produced, although their practical valorization would require additional purification steps. Overall, the study demonstrates that EOP can serve as a viable feedstock for activated carbon production via autothermal pyrolysis, offering a sustainable route for waste valorization while ensuring favorable energy balances.

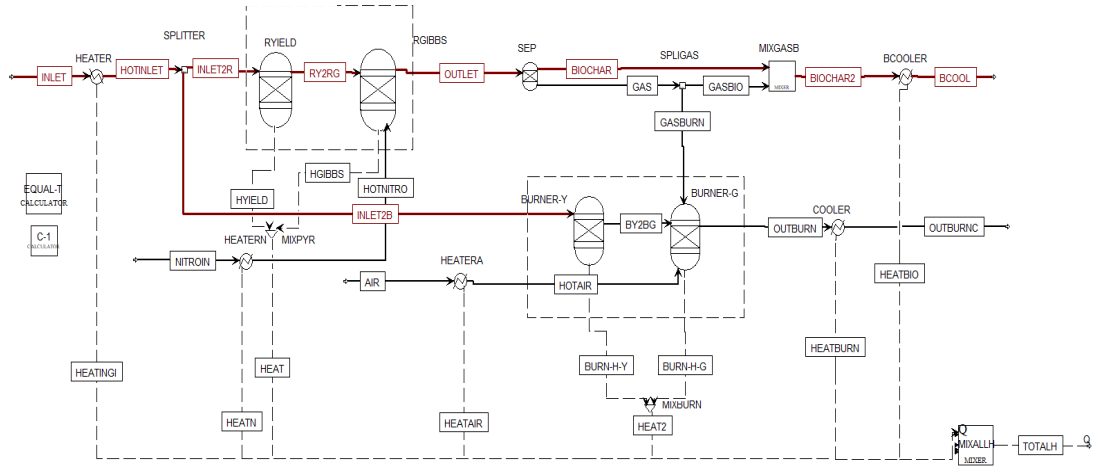

Fig. 1. Main flowsheet diagram of the process (case 1) as viewed from Aspen Plus V15.

Acknowledgements: This work was supported by national funds supported this work through FCT/MCTES (PIDDAC): CIMO, UIDB/00690/2020 (DOI: 10.54499/UIDB/00690/2020) and UIDP/00690/2020 (DOI: 10.54499/UIDP/00690/2020); and SusTEC, LA/P/0007/2020 (DOI: 10.54499/LA/P/0007/2020). Ana Paula Ferreira acknowledges the doctoral Grant PRT/BD/153090/2021 financed by FCT and with funds from NORTE2020, under MIT Portugal Program. Jose L. Diaz De Tuesta acknowledges financial support through the grants 2022-T1/AMB-23946 and CNS2024-154264 funded by *Comunidad de Madrid* and *Agencia Estatal de Investigación*, respectively.

[1]Ferreira, A.P.; Baldo, A.P.; Silva A.S.; Natal, A.P.S.; Bezerra A.J.B.; Diaz de Tuesta, J.L.; Marin, P.; Peres, J.A.; Gomes, H.T. *J. Water Process Eng.* **2025**, *75*, 107914.

EES - D4- P11
Synthesis and characterization of lithium metal phosphates in various solvents

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In this study, lithium metal phosphates (LMPs) are synthesized and characterized using cobalt(II), manganese(II), and nickel(II) nitrate salts. The synthesis is performed using the molten salt-assisted self-assembly (MASA) method. This approach involves forming a lyotropic liquid crystal phase from a clear lithium nitrate ($LiNO_3$), transition metal nitrates ($[M(H_2O)_6](NO3)_2$), phosphoric acid (H_3PO_4), and surfactant (Pluronic P123) alcohol solution. If a resulting solution contains a solid phase, the mixture is subjected to centrifugation to separate into supernatant and solid phases, which are then analyzed using various techniques.

The clear solutions are prepared with molar ratios of 1:30:30:30 (P123:Li(I):M(II):H_3PO_4). Then, they are drop-cast onto glass slides and heated between 300-700°C to form powders. The resulting mesoporous solids formed after calcination are characterized using XRD, SEM, N_2 adsorption-desorption, and ATR-FTIR techniques.

Up to 500°C, the solution, supernatant, and solids remain amorphous but crystallize at higher temperatures. ATR-FTIR analyses reveal that the nitrates in the solution and supernatant decompose by reacting with phosphoric acid. SEM analyses show that the solids became more porous after calcination. N_2 adsorption-desorption analysis indicates that the pore volume and size vary depending on the temperature.

We found that the precipitates form metal pyrophosphates, while the supernatants form LMPs; the supernatants form $LiMnPO_4$, $LiCoPO_4$, and $LiNiPO_4$ in the olivine phase; the precipitates of Mn(II) solution is crystalline $MnPO_4 \cdot H_2O$ that is converted to $Mn_2P_2O_7$ at temperatures above 400°C. The Ni(II) and Co(II) precipitates form $M_2P_2O_7$. Additionally, cyclic voltammetry experiments were conducted at different KOH concentrations. The $LiNiPO_4$ obtained from 1-butanol and coated onto FTO exhibit greater stability and electrochromic properties during water oxidation.

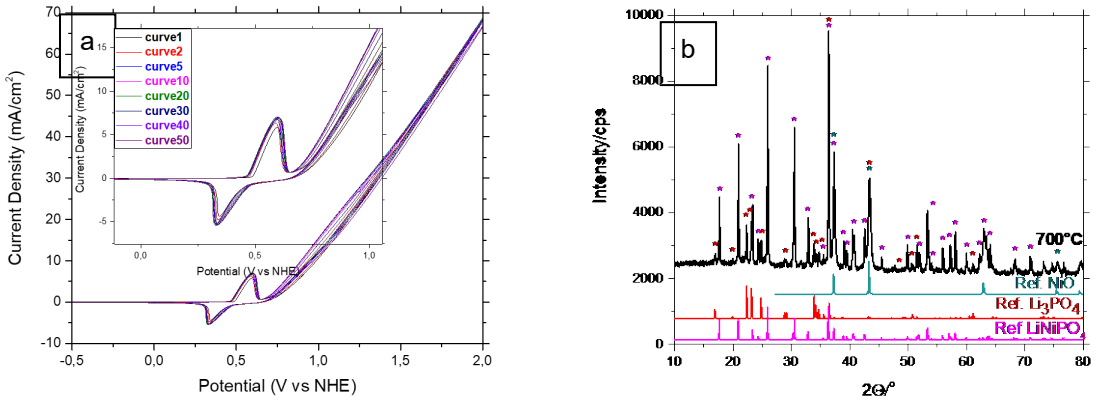

Fig. 1. a) $LiNiPO_4$ electrode (prepared from 1-Buthanol supernatant and calcined at 400 °C), and b) $LiNiPO_4$ supernatant with various crystalls.

[1]Albayrak, C.; et al. *Chem. Eur. J.* **2012**, *18*, 4130.
[2]Uzunok, I.; et al. *ChemPlusChem.* **2019**, *84*, 1544–1553.

EES - D4- P12

Integrated zeolite membrane and Cu-ZnO-Al_2O_3 catalyst for intensified CO_2-to-methanol conversion

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The hydrogenation of CO_2 to methanol is an attractive pathway for carbon utilisation and sustainable fuel production. However, in conventional fixed-bed reactor, Initiate water formation shifts the equilibrium backward, lower methanol yield, and accelerate catalyst deactivation. A membrane reactor integrating a water-selective membrane with methanol synthesis catalyst offers a promising solution for continuously removing water, enhancing conversion via Le Chatelier's principle. This work focuses on development of zeolite membrane and Cu-Zn-Al_2O_3 catalyst and their integration into single membrane reactor system.

The membrane including silicate, zeolite A, zeolite 3A, and ZSM-5 were synthesised on porous alumina support using a secondary growth hydrothermal method. Membrane performance was evaluated through a single and mixed gases permeation experiments, emphasizing H_2O selectivity. It is found that silicate membrane showed lower water transport due to their hydrophobic nature, while ZSm-5 membrane displayed moderate separation behaviours.

Cu-ZnO-Al_2O_3 Catalyst was prepared via co-precipitation with varying total metal loading (10-70 wt.%). Catalytic activity was tested in fixed-bed reactor after calcination and H_2 reduction. Results indicate that metal loading significantly influence methanol productivity: excessive loading led to particle agglomeration and reduced activity whereas intermediate loading improved copper dispersion and enhance CO_2 conversion. Finally, the optimized membrane and catalyst were integrated into a membrane reactor. Reactor performance was evaluated at varying temperature, pressure, and feed flow rate in terms of CO_2 conversion, methanol selectivity and water permeation. Integrated operation showed clear potential for improved methanol yield compared to conventional system.

Acknowledgements: The authors acknowledge the support of the Dept. of Chemical Engineering and Technology, IIT (BHU) Varanasi, for providing research facilities.

[1]Gallucci, F.; Fernandez, E.; Corengia, P.; van Sint Annaland, M. Chem. Eng. Sci. 2013, 92, 40–66.
[2]Behrens, M. et al. Science 2012, 336, 893–897.

EES - D4 - P13

Kinetic analysis and multiscale hydrolysis of reinforced PET and PBT plastics: Innovative process configurations for enhanced monomer recovery

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Plastic use has risen since the mid-20th century due to its durability and versatility. For industrial applications, plastics like Poly(ethylene terephthalate) (PET) and Poly(buthylene terephthalate) (PBT), are often combined with glass fiber to improve mechanical properties. Consequently, recycling these materials is challenging and solvolysis can be considered a viable alternative.[1] The references regarding the chemical recycling of reinforced industrial plastics are scarce, particularly PBT, and effect of glass fiber was not investigated. The novelty of this work lies in a multiscale study of hydrolysis of these materials along with proposing new process configurations to enhance the monomers recovery. First, a kinetic study was performed using data from differential scanning calorimetry (DSC) with high pressure crucibles, a much faster alternative that uses less energy and fewer reagents than batch-scale experiments. We were able to estimate activation energy, identify main trends and eventual side reactions, and the impact of glass fiber on polymeric matrix. Although glass fiber can slightly modify the kinetic parameters, the results from batch experiments showed a small difference in polymer conversion, without impact on the monomer recovery. Furthermore, the batch reactions allowed for the characterization of products obtained and, in the case of PBT, the diol monomer (1,4-butanediol (1,4-BD)) recovery was lower than 10 %, regardless of the presence of glass fiber. To increase the 1,4-BD recovery, we performed hydrolysis in presence of KOH. Under these conditions, the dehydration of 1,4-BD is prevented and its recovery increased from 10% to approximately 80%. For the PET+30%GF it was demonstrated that recycling the process water associated with the washing of solid residues can increase more than 3x the initial concentration of EG without an impact on polymer conversion, as represented on Figure 1.

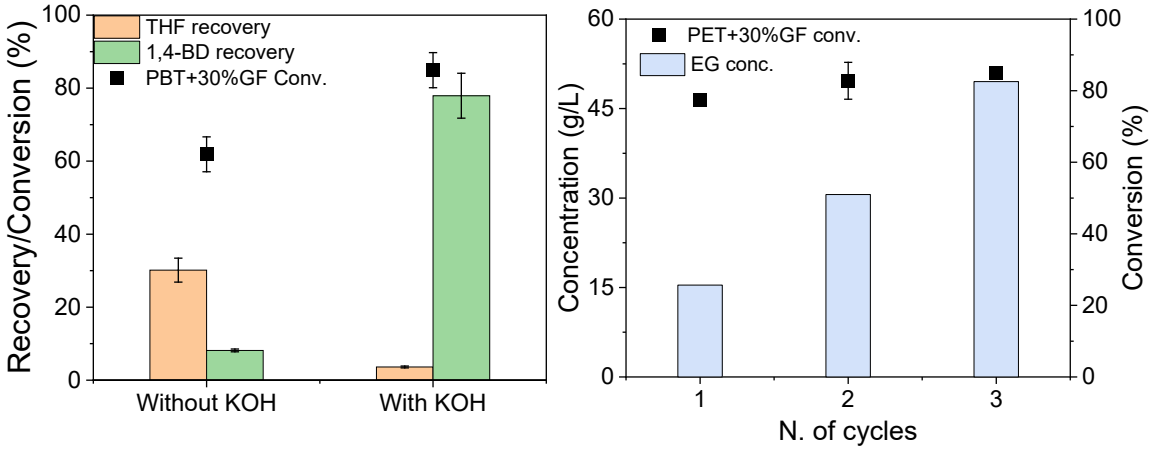

Fig. 2. Conversion and monomer recovery for various strategies to enhance monomer recovery in PBT (left) and PET (right) reinforced with 30% glass fiber.

[1]Rubio Arias, J. J. and Thielemans, W. *Polymers* **2022**, *14* (23), 5171.

EES - D4 - P14
Electroreduction of CO_2 to C1 and C2 products on dual active sites

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Electrochemical CO_2 reduction (eCO_2RR) is a promising method for transforming CO_2 emissions into useful multicarbon products. This study involved the synthesis and evaluation of CuS/ZnS nanocomposites with varying compositions (CuS: ZnS = 1:1, 2:1, and 1:2) in both H-type and flow-cell electrolyzers. The catalyst with a 2:1 CuS/ZnS ratio (S2) exhibited excellent performance, with a Faradaic efficiency (FE) of 60% for C_1 products and approximately 20% for C2 products (C_2H_4) at a current density of −280 $mA \cdot cm^{-2}$ in the flow-cell configuration. The flow-cell arrangement significantly enhanced catalytic activity, suppressed hydrogen evolution, and increased selectivity for CH_4 and C_2H_4 at greater negative potentials. Augmented ethylene production was ascribed to Cu-rich active sites promoting efficient C–C coupling and increased CO_2 accessibility at gas diffusion electrodes (GDEs), corroborated by low charge-transfer resistance (~1 $\Omega \cdot cm^2$). This work emphasizes the pivotal importance of catalyst composition and reactor design, showcasing the 2:1 CuS/ZnS catalyst in a flow-cell format as a scalable and effective method for sustainable CO_2 conversion to multicarbon fuels. Density functional theory (DFT) calculations further validated the experimental results by revealing favorable adsorption energies and interactions between the CuS/ZnS catalyst and key intermediates in the CO_2 conversion process.

EES - D4- P15

Efficient dissolution and selective recovery of gold from electronic waste using a recyclable ionic medium

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The significant socio-economic and technological importance of gold necessitates sustainable supply to meet the continuously rising demand. As the demand rises, recovering gold from secondary sources has become increasingly important, highlighting the need for environmentally and economically sustainable extraction processes.[1-5] In this study, gold was efficiently and rapidly leached quantitatively as Au(III) halometalate (Cl/Br) complexes and selectively recovered (~100%) in eight different hydrophobic ionic liquids (ILs) based on pyridinium, pyrrolidinium, and imidazolium at room temperature from both mixed metals solution and electronic waste (e-waste). ILs were recovered after extraction, and used for another two cycles for dissolution and recovery of gold thus demonstrating the economic sustainability of the developed process. Moreover, a techno-economic analysis of the method reveals attractive numbers for gold recovery, even without recycling of ILs. The background for the selective chemistry was studied comprehensively using diverse analytical techniques, complemented by density functional theory (DFT) calculations, and life cycle analysis (LCA). Furthermore, single crystal X-ray diffraction and DFT calculations revealed that non-covalent interactions between the cationic part of the IL and Au(III) halide are key for selective gold separation. The LCA study demonstrates that the process can lower CO_2 emissions by ~84.4% compared to conventional gold mining under the current Indian energy mix, with the potential for an almost complete emissions reduction (~99.9%) if powered by solar energy. The developed process is expected to pave the way for economic and environmentally sustainable recycling of multi-metals from e-waste.

Acknowledgements: A.N. and K.M.P. acknowledges the Marie Skłodowska-Curie Actions–European Commission post-doctoral grant (REWCHEM, Grant agreement ID: 101152892) and Sustain-a-Print project (Grant agreement ID: 101070556) from European Commission for research funding. P. B. acknowledges, Ramón y Cajal grant from Spanish State Investigation Agency (Grant no. J03416).

[1]Nag, A.; Islam, M. R.; Pradeep, T. *ACS Sustainable Chemistry & Engineering* **2021**, *9*, 2129-2135.
[2]Nag, A.; Singh, M. K.; Morrison, C. A.; Love, J. B. *Angew. Chem. Int. Ed.* **2023**, *62*, e202308356.
[3]Nag, A.; Morrison, C.; Love, J. *ChemSusChem* **2024**, *17*, e202301695.
[4]Nag, A.; Morrison, C. A.; Love, J. B. *ChemSusChem* **2022**, *15*, e202201285.
[5]Nag, A.; Qurashi, A.; Morrison, C. A.; Moth-Poulsen, K.; Pradeep, T.; Love, J. B. *Coord. Chem. Rev.* **2026**, *548*, 217186.

EES - D4 - P16

Comparative assessment of microplastic accumulation in upper catena fisheries of the Kothmale reservoir, Sri Lanka

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Microplastic (MP) pollution has rising threats in environmental safety. This study aims to address the gap in MP contamination of upper catena freshwater fish in Sri Lanka by examining MP accumulation in three fish species, *Rasbora microcephalusv, Glossogobius giuris and Puntius dorsalis* inhabiting in the Kothmale reservoir, Sri Lanka. Samples (n = 75) were collected from the local fishermen in July and October 2024. Samples were digested in 10% KOH, stained with Nile red, identified under a stereomicroscope, and further by the μ-FTIR spectroscopy. Overall, MPs were detected in 52% tracts (n =39) and 37.3% gills (n=28). In *R. microcephalusv,* the mean MP abundance was 0.039 ± 0.042 items/gram. Fibers are dominated (64%), while most frequent MP size range (0.1 - 1 mm) accounted for 77.27%. Predominant colors of MPs were blue, black, and red, with blue at 56%. In *G. giuris,* mean MP abundance was 0.012 ± 0.010 items/gram. Fibers have dominated (88%) with the most MPs sized 0.1 - 1 mm (52.38%) in range. Blue, black and red colours MPs were prevailed, with blue colour comprising in 46%. In *P. dorsalis,* the mean MP abundance was 0.062 ± 0.071 items/gram with fibers constituting 63%. Most MPs were sized 0.1 - 1 mm (90.70 %), with blue making up 74%. The chemical composition of extracted MPs from fish samples revealed Polyolefin fibers, HDPE, Polypropylene (PP). There was a significant difference between three species ($p < 0.05$). Findings indicate broad MP pollution, needing better monitoring to prevent harm.
Keywords – Microplastic, Rasbora microcephalus, Glossogobius giuris, Puntius dorsalis, μ-FTIR

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[1]Athukorala, A., Amarathunga, A. a. D., De Silva, D. S. M., Bakir, A., McGoran, A. R., Sivyer, D. B., Dias, B. C. G., Kanishka, W. S., & Reeve, C. (2024). Pervasive Microplastic Ingestion by Commercial Fish Species from a Natural Lagoon Environment. *Water*, *16*(20), 2909. https://doi.org/10.3390/w16202909.
[2]Dias, B. C. G., Amarathunga, A. a. D., De Silva, D. S. M., Bakir, A., McGoran, A. R., Athukorala, A., Sivyer, D. B., Reeve, C., & Maddumage, M. D. S. R. (2024). The Ecological Implication of Microplastic in Crabs from a Tropical Lagoon: Ingested Microplastic in Mud Crab Scylla serrata. *Water*, *16*(23), 3534. https://doi.org/10.3390/w16233534

EES - D4 - P17

Tailored-shell hollow TiO_2 spheres with reduced tortuosity for fast-charging anode

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Growing attention has been paid to next-generation anode materials beyond graphite. Titanium dioxide (TiO2) has attracted considerable interest due to its structural stability and natural abundance; however, its practical application is limited by sluggish Li^+ transport arising from the dense arrangement of TiO_6 octahedra.

In this study, we present a structurally engineered TiO2 anode featuring a hollow mesoporous architecture composed of nanoscale anatase particles. The design integrates two key advantages: (i) a shortened Li+ diffusion pathway enabled by thin shells and (ii) enhanced electrolyte accessibility through interconnected mesopores. The hollow interior further provides additional active interfaces, allowing bidirectional ion transport across the shell.

The hollow TiO2 spheres were synthesized via a template-assisted route, where sub-20 nm TiO2 nanoparticles prepared by a sol-gel process were assembled onto carbon nanospheres, followed by removal of the sacrificial carbon core. By precisely controlling shell thickness, the ion transport resistance within the electrode was significantly reduced while suppressing isolated pore formation. As a result, a Li+ diffusion coefficient of 3.22x10-11 cm2 s-1 was achieved, representing a ~40-fold enhancement compared to bulk TiO2.

Electrochemically, the optimized TiO2 anode delivered 0.66 mol Li per mol TiO2 at 0.5C and retained 67% of its capacity even at 10C, demonstrating excellent rate capability. In addition, long-term cycling at 20C exhibited a capacity retention of 85.9% over 1000 cycles, indicating outstanding structural robustness under high-rate conditions. When paired with a LiFePO4 cathode, the full cell showed a rate performance of 60% (2000 vs. 50 mA g-1, surpassing that of conventional bulk TiO2 systems.

These results highlight that rational control of mesostructure and shell thickness is an effective strategy to overcome intrinsic kinetic limitations of TiO2, providing a viable pathway toward high-power lithium-ion batteries.

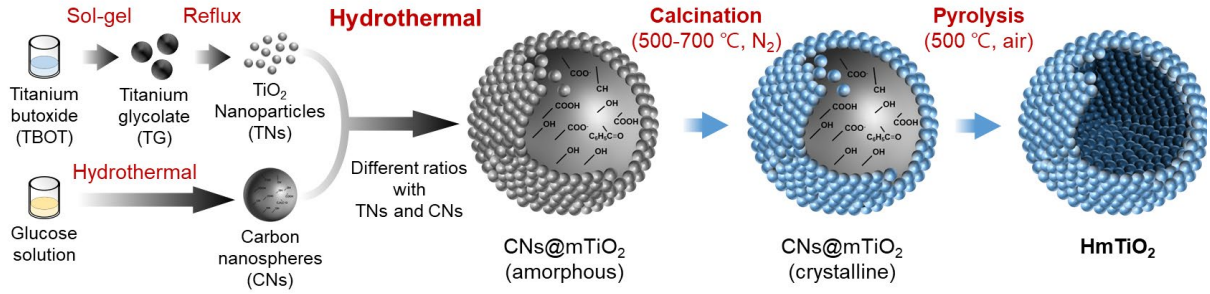

Fig. 1. Schematic of the synthesis of hollow mesoporous TiO_2 spheres ($HmTiO_2$) using carbon nanosphere as a sacrificial scaffold, onto which TiO_2 nanoparticles were assembled, followed by calcination and pyrolysis.

This work was supported by the National Research Foundation of Korea (NRF) funded by the Korean government (Ministry of Science, ICT & Future Planning) (NRF-2021R1A4A2001658; NRF-2022R1A2C1009922).

EES - D4 - P18

Regulating redox sites for photocatalytic phenylcarbinol conversion and H_2 production on lattice-matched Schottky junction

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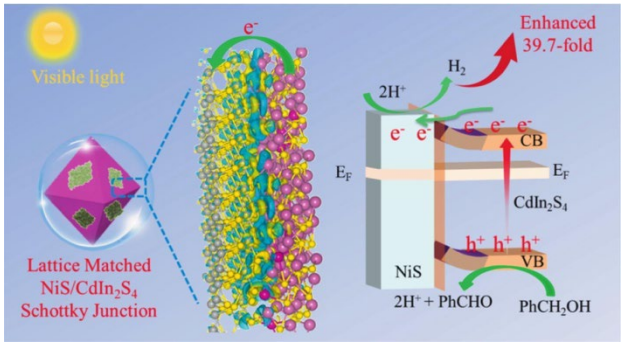
The photocatalytic coupling of selective phenylcarbinol oxidation with hydrogen evolution has attracted considerable attention as a promising dual-functional reaction system. Herein, a lattice-matched 2D/3D NiS/$CdIn_2S_4$ (NiS/CIS) Schottky heterojunction is rationally designed for efficient dual-functional photocatalysis under visible light. Structural analyses confirm the uniform deposition of NiS nanosheets on octahedral CIS with a lattice mismatch below 5%, ensuring coherent interfacial contact. The optimal 3% NiS/CIS composite exhibits exceptional hydrogen and benzaldehyde production rates of 2636.4 and 2717.6 μmol g^{-1} h^{-1}, respectively—representing enhancements of 39.7 and 38.0 times over pristine CIS. The catalyst also demonstrates remarkable stability, retaining over >99.0% activity after six cycles. Mechanistic studies reveal that the Schottky junction facilitates spatial separation of photogenerated carriers: electrons migrate to NiS, prolonging charge carrier lifetimes and lowering the hydrogen evolution overpotential, while holes accumulate on CIS that facilitated phenylcarbinol adsorption to drive selective phenylcarbinol oxidation via a carbon-radical pathway. This work provides a viable approach for designing efficient bifunctional photocatalysts through lattice-matched interface engineering.



Graphic abstract: Lattice-matched 2D/3D NiS/$CdIn_2S_4$ Schottky junction was designed and prepared for efficiently separation and guided transfer of photogenerated electrons and holes into targeted redox sites, leading to efficiently and sustainably dual-functional photocatalysis.

EES - D4 - P19
Revealing battery interface chemistry with spectroscopy

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Interfaces and interphases largely determine the lifetime, performance, and safety of modern commercial lithium-ion batteries. Yet, probing the formation and chemical composition of these thin and unstable "solid-electrolyte interphases" (SEIs) remains very difficult. As a result, the battery cell conditioning protocols used in industry to establish a "good SEI" are often lengthy and expensive, guided by institutional knowledge and historical practice, rather than chemical considerations. In this work, we present an analytical toolkit that can be used to track the generation and evolution of these interphases: Operando shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS), and post-mortem Nuclear Magnetic Resonance (NMR) spectroscopy. The methods are demonstrated with standard 2032-format coin cell batteries constructed with commercial lithium-ion battery electrodes and a model electrolyte. Data will be presented addressing a longstanding dispute[1-4] regarding the chemical composition of an SEI layer forming on a graphite anode with an electrolyte containing ethylene carbonate. The origin of this dispute is traced to moisture contamination and the formation of metallic lithium depositions, both of which were found to alter the chemical structure of the carbonate-based decomposition products that dominate the SEI. It is hoped that these insights will aid in the development of better batteries and cell conditioning protocols in the future.

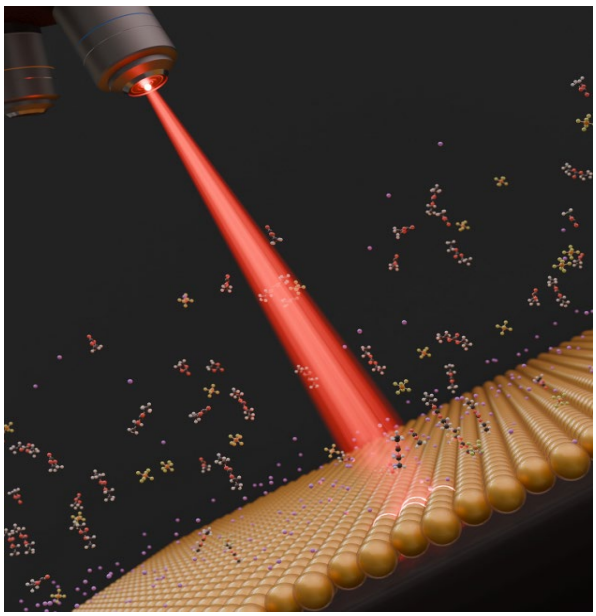

Fig 1. Illustration of the SHINERS method on a graphite anode.

[1] D. Aurbach et al., *J. Electrochem. Soc.,* **1987**, *134(7)*, 1611-1620.
[2] M. Nie et al., *J. Phys. Chem. C,* **2013**, *117*, 1257-1267.
[3] L. Wang et al., *Nat. Chem.,* **2019**, *11*, 789-796.
[4] A. Gajan et al., *ACS Energy Lett.,* **2021**, *6*, 1757-1763.

EES - D4 - P20
Investigation of MOF Derived NASICONs for capacitive deionization application

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Global water scarcity necessitates the development of highly energy-efficient desalination technologies. While Capacitive Deionization (CDI) stands out as a sustainable alternative, the system's efficiency is directly dependent on the electrochemical properties of the electrode materials[1]. This study investigates the synthesis and performance of NASICON-type structured materials derived from Metal-Organic Frameworks (MOFs) for the selective removal of Na ions from brackish water. By using MOFs as sacrificial templates, a hierarchical porous architecture that facilitates rapid ion diffusion and offers a high surface area has been successfully designed. Through the carbonization of MOF precursors followed by thermal treatments, a stable NASICON framework (e.g., $Na_3Zr_2Si_2PO_{12}$ or similar analogs) integrated into a conductive carbon matrix has been obtained. This unique structure preserves structural integrity while simultaneously leveraging the high theoretical capacity of faradaic materials. Electrochemical evaluations, including cyclic voltammetry and galvanostatic charge-discharge tests, demonstrate that MOF-derived NASICON electrodes exhibit higher salt adsorption capacity (SAC) and faster desalination kinetics compared to conventional activated carbon electrodes. This performance improvement is based on the synergistic effect between the intercalation pseudocapacitance of the NASICON phase and the high conductivity of the MOF-derived carbon. In this study, MOF crystals obtained from titanium salt and dihydroxyterephthalic acid will be converted into NASICON. And the prepared electrodes using for desalination of seawater. This research presents a promising strategy for the design of next-generation, high-performance electrodes for efficient water treatment.

Acknowledgement: This work was supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) under grant number 223M289.

[1]Kumar, S.; Aldaqqa,N.M.; Alhseinat, E.; Shetty, D. *Angew. Chem.* **2023***, 135,* e202302180

EES - D4 - P21

Proposal for restriction on difluoromethylene substances aka "universal PFAS restriction": Chemical analysis

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Currently considered proposal for restriction of "Per- and polyfluoroalkyl substances (PFAS)"[1], does not define the restricted compounds correctly. A reasonably correct chemical name could be, for example, "substances with at least one difluoromethylene group, not connected to H, Cl, Br of I".
The name "PFAS" is confusing: a substance with a -CF_2- may be not an "alkyl" substance (Fig. 1).
The formula for exclusion of certain "PFAS" from the restriction – "A substance that only contains the following structural elements is excluded from the scope of the proposed restriction: CF3-X or X-CF2-X', where X = -OR or -NRR' and X' = methyl (-CH3), methylene (-CH2-), an aromatic group, a carbonyl group (-C(O)-), -OR'', -SR'' or –NR''R''', and where R/R'/R''/R''' is a hydrogen (-H), methyl (-CH3), methylene (-CH2-), an aromatic group or a carbonyl group (-C(O)-)." - is as complex as controversial and, therefore, hardly of any use: each mentioned substance of formula X-CF_2-F can be considered as X-CF_3 or as X-CF_2-F', with the opposite outcomes (Fig. 1).
For an organic chemist, it is hard to understand why only ethers of primary alcohols are suggested for exclusion, while equally degradable ethers of secondary and tertiary alcohols – not (Fig. 1).
For an environmental chemist, it is hard to accept more severe restrictions on substances with difluoromethylene group, and milder restrictions on substances with "more perfluorinated" trifluoromethyl group (Fig. 1).
These inconsistencies originate from the report[2] with explanation of "PFAS" for non-experts, which was later presented as "A New OECD Definition for Per- and Polyfluoroalkyl Substances" in a non-peer reviewed paper[3] and laid foundation for the restriction proposal.
Use of scientifically correct description of substances proposed for restriction, instead of excerpts from non-peer reviewed papers should be recommended in the future, to avoid science-based criticism and enhance credibility of environmental protection initiatives.

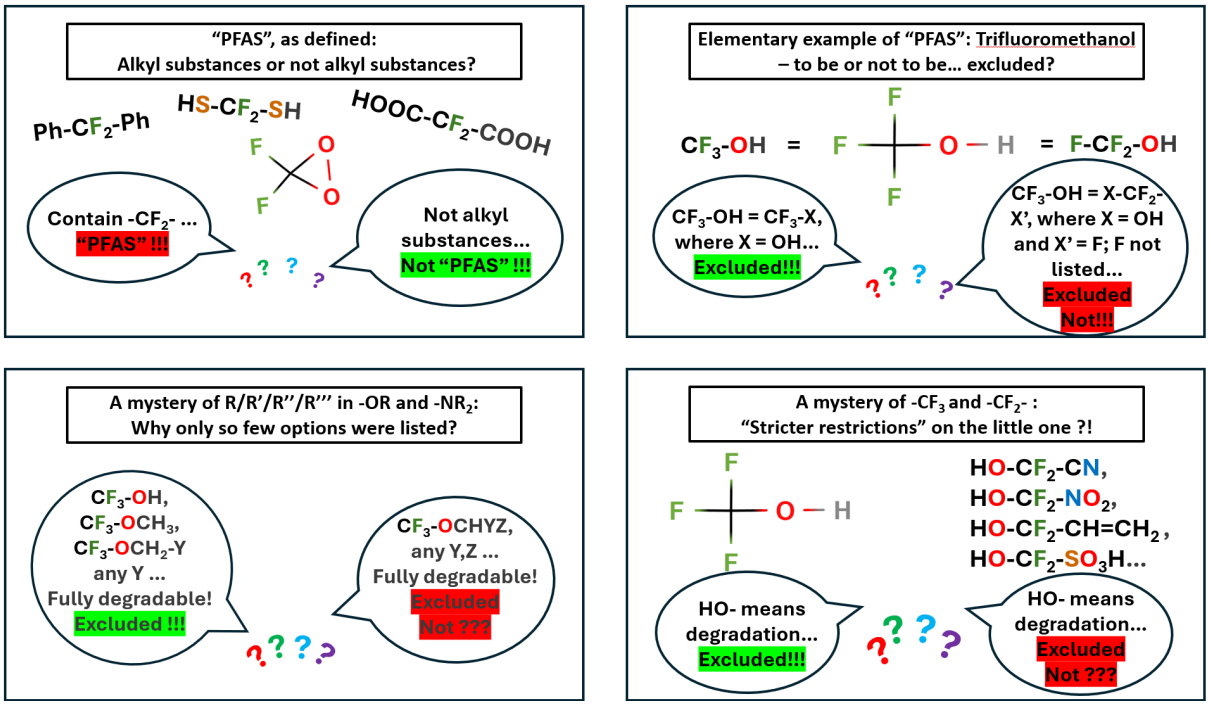

Fig. 1. Graphical representation of major inconsistencies of the restriction proposal.

[1]Registry of restriction intentions until outcome - ECHA
[2]OECD **2021**, Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance, OECD Series on Risk Management, No. 61, OECD Publishing, Paris.
[3]Wang, Z. et al. Am. Chem. Soc. 1961, 83, 449–453. Environ. Sci. Technol. 2021, 55, 15575–15578

EES - D4 - P22

Electronic structure engineering via atomic W doping in NiO/Cr_2S_3 nanotube heterostructures for enhanced overall water splitting

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The development of durable and highly active non-precious electrocatalysts for hydrogen and oxygen evolution reactions (HER/OER) is essential for advancing hydrogen energy technologies. Herein, we report a vertically aligned W-doped NiO/Cr_2S_3 nanotube heterostructure grown on nickel foam (denoted as $W–NiO/Cr_2S_3/NF$) via a combined electrodeposition and etching strategy. The incorporation of W atoms effectively modulates the electronic structure of the NiO/Cr_2S_3 interface, leading to enhanced intrinsic catalytic activity. Density functional theory (DFT) calculations reveal that the HER activity is governed by the electronic states of the active valence dz^2 orbitals. W doping introduces antibonding states with an optimized occupancy, resulting in near-ideal hydrogen adsorption energetics. As a result, the $W–NiO/Cr_2S_3/NF$ electrode exhibits outstanding bifunctional catalytic performance for overall water splitting, requiring a low cell voltage of 1.58 V at 10 mA cm^{-2}. Moreover, it demonstrates excellent durability over 50 h in 1.0 M KOH, surpassing the performance of commercial Pt/C and IrO_2 catalysts. These findings highlight the effectiveness of atomic-level doping in tuning electronic structures and provide a promising strategy for designing high-performance electrocatalysts for sustainable hydrogen production.

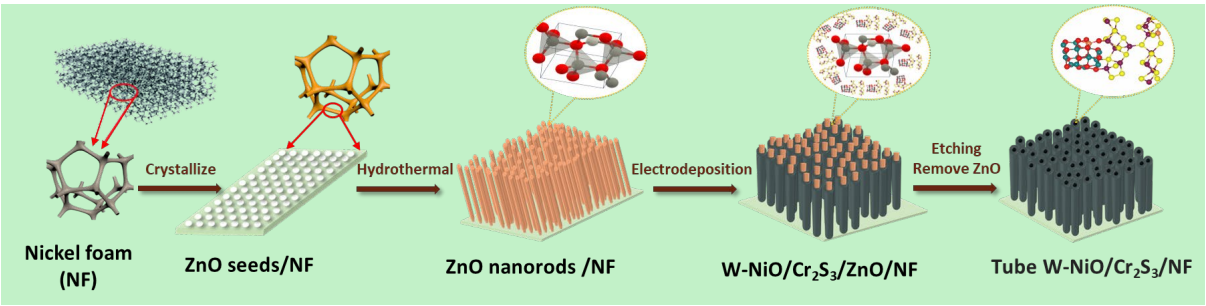

Fig 1. Material Fabrication: W-doped NiO/Cr2S3 hollow heterostructure on nickel foam

Acknowledgement: This work was supported by the Korea-Vietnam Joint Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2026-16063221). This research was also supported by the Regional Innovation System & Education (RISE) program, funded by the Ministry of Education (MOE) and the Jeonbuk State, Republic of Korea (2025-RISE-13-JBU).

[1]Hoa, V. H.; Tran, D. T. Tran; Nguyen, D. C.; Kim, D. H.; Kim, N. H.; ; Lee, J. H. Adv. Funct. Mater, **2020**, 30, 2002533.
2Mai, M.; Hoa, V.H.; Prabhakaran, S.; Dao, H. T.; Kim, D.H.; Appl. Catal. B Environ. Energy, **2025**, 361, 124641.

EES - D4 - P23
Ti/Fe-based MOF photocatalysts for efficient solar-driven dye removal

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Marmara University, Faculty of Engineering, Chemical Engineering Dept., Türkiye

The discharge of dye-containing wastewater poses a significant environmental challenge due to its toxicity, persistence, and resistance to conventional treatment methods. In this context, solar-driven photocatalysis has emerged as a sustainable and energy-efficient alternative for the degradation of organic pollutants [1, 2]. This study focuses on the synthesis and evaluation of Ti/Fe-based metal–organic framework (MOF) photocatalysts for the efficient removal of dye contaminants under solar irradiation.
Ti-MOF, Fe-MOF, and bimetallic Ti/Fe-MOF structures with different metal ratios were synthesized and systematically characterized in terms of their structural, morphological, and optical properties. The photocatalytic performance of the prepared materials was investigated using methylene blue as a model dye pollutant under simulated solar light.
To optimize the degradation process, a Taguchi L16 experimental design was employed. Four key factors—catalyst type, catalyst loading, initial dye concentration, and reaction time—were examined at four levels each. This approach enabled the identification of the most influential parameters affecting photocatalytic efficiency with a reduced number of experiments. The experimental results were statistically analyzed using analysis of variance (ANOVA) to determine the significance and contribution of each factor. The findings highlight the potential of Ti/Fe-based MOF photocatalysts as promising candidates for sustainable wastewater treatment applications.

[1]Kerkez, Ö.; Boz, İ. *Chem. Eng. Commun.* **2015**, *202*, 534–541.
[2]Rauf, M. A.; Salman Ashraf, S. *Chem. Eng. J.* **2009**, *151*, 10–18.

EES - D4 - P24
Fine-tuning the supercapacitor's performance with EPR spectroscopy

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[2]Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania

Supercapacitors (SCs) are promising energy storage devices, where the electrode materials are key components; selecting the right electrodes is crucial to their specific power and energy storage performance. 3D carbon materials derived from MOFs and impregnated with ZnO are used as electrode materials in hybrid SC devices. Here, their electrical properties are enhanced by controlling and tailoring the size, shape, defects, interfacial phenomena, and porosity of the materials' nanostructures. The high-sensitivity EPR spectroscopy method is used to characterize defect structures, including carbon-related defects and oxygen-vacancy-related defects, in ZnO. The characterization by spectroscopic techniques on the surface and interface of the electrodes and their influence on the electronic, optical, and electrical properties of the nanocomposites is carried out to improve the properties of the material, so that new SC electrodes in a solid-state configuration using a 3D-carbon structure/ZnO are obtained to improve the energy storage capacity.

Acknowledgement: The authors acknowledge the support of a grant from the Ministry of Research, Innovation and Digitization, CNCS—UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0048, within PNCDI IV.

EES – D4 - P25
Valorisation of waste tea leaves and egg shells in carbon nanodot synthesis

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[1]Marmara University, Chemical Engineering Dept., Turkiye

Utilization of food waste as renewable raw materials offers vast opportunities in terms of tbioeconomy and the reduction of associated environmental concerns1. Concordantly, significant research effort has been put into the valorisation of food waste to create 'added value products' such as carbohydrates, essential oils, enzymes[2], and even nanomaterials, particularly carbon nanoparticles and carbon quantum dots (CNP, CQD)[3]. The exquisite optical, electrical and chemical properties of CQDs facilitate their utilization in a variety of applications ranging from sensors, and bio-imaging to food packaging and water treatment[3].
In this study, waste tea leaves and eggshells were utilized as low-cost raw materials for the synthesis of carbon nanodots (CNDs). While tea wastes served as the primary carbon source due to the inclusion of carbonaceous organic compounds, eggshells acted as a dopant and modifier due to the abundancy of calcium carbonate in its structure.The synthesis was conducted solvothermally in a deep eutectic solvent composed of urea and glycerol. The effects of solvent composition, reaction temperature and precursor ratio on CND properties and yield were evalutaed. The chemical, optical and moprhological characteristics of CNDs were determined using UV–Vis absorption spectroscopy, fluorescence spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and transmission electron microscopy (TEM).
The results verified nanoparticle formation with photoluminescent character. Reaction temperature was identified as the most effective parameter. The presence and density of hydroxyl and carboxyl surface functional groups were also affected, which determined water solubility. Moreover, increased ratio of eggshells led to enhanced optical properties.

[1]Ansari, S.A.; Kumar, T.; Sawarkar, R.; Gobade, M., Khan, D., Singh, L. *J. Env. Man.* **2024**, 364,121439.
[2] Sarker, A.; Ahmmed, R., Ahsan, S. M.; Rana, J.; Ghosh, M.K.; Nandi R. *Sustainable Food Technol*. **2024**, 2, 48-69.
[3]Magri, P.; Franchetti, P.; Gaumet J.-J.; Maxit, B.; Diliberto, S.; Pierrat, P. *Appl. Sci.* **2024**,14, 8807.

EES - D4 - P26
Bioinspired catalysts for photoelectrochemical solar energy conversion

Corentin Pigot [1], Simona Porzio[2], Sergii Shyliin[3]

Employing renewable energy for the production of green fuels, using atmospheric CO_2 as building block, is one of today's greatest technological challenges. Fossil resources have had a monumental impact on the quality of life during the past century, with an abundance of commodities such as fuels and chemicals being produced for the enrichment of everyday life. High shares of fuels from non-fossil origin are needed by 2050, if the target for net-zero emissions should be reached [1]. Nowadays, eFuels can be produced by electrocatalytic water oxidation and CO_2 reduction. However, rare and expensive metals are required, and catalysts have low stability and are sensitive to poisoning. In addition, production of eFuels relies on the external electricity input from intermittent sources [2].
In this project, **we are working on a technology inspired by photosynthesis, where solar energy is converted directly to fuels without secondary energy carriers**, such as external renewable electricity generated *e.g.* with separate photovoltaics (PV). In the process of direct solar-to-fuel (STF) production proposed here, the energy from sunlight is used to oxidize water into oxygen (O_2), and released electrons are used to reduce CO_2 to various fuel targets. **Our vision** is to develop a photoelectrochemical (PEC) cell technology for direct STF conversion. **The unique feature of this project is the combination of molecular catalysts for water oxidation and CO_2 reduction with light absorbing semiconductors.**
In this system the catalysts are made out of Cu, Fe or Ni which are extremely robust in water in both low and high oxidation states [3,4]. In combination with a relatively low water oxidation overpotential [4], this makes this family of materials excellent WOCs, which hold the promise to compete with the well-known Ru- and Ir-based catalysts [4].

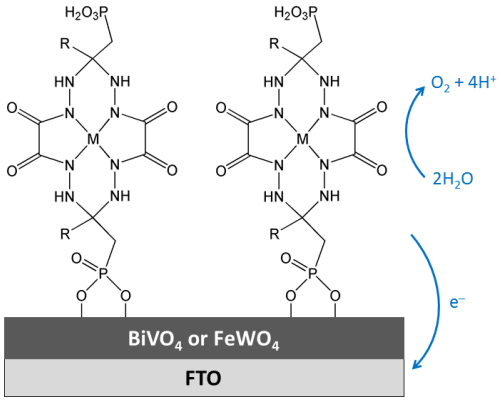

Figure 1. *Photoanode containing new tetrahydrazido complexes as WOCs (M = Mn, Fe, Cu, Fe).*

[1] Communication from the European Commission to the European Parliament and the Council, "*Sustainable Carbon Cycles*", **2021**.
[2] Lee D. K., Lee D., Lumley M. A., Choi K. S.. *Chem. Soc. Rev.*, **2019**, *48*, 2126.
[3] Shylin S. I., Pavliuk M. V., D'Amario L., Mamedov F., Sá J., Berggren G., Fritsky I. O., *Chem. Commun.*, **2019**, 55, 3335.
[4] Shylin S. I., Pogrebetsky J. L., Husak A. O., Bykov D., Mokhir A., Hampel F., Shova S., Ozarowski A, Gumienna-Kontecka E., Fritsky I. O., *Chem. Commun.*, **2021**, 57, 11060.

EES - D4 - P27

Atmospheric microplastics in a Brazilian elementary school and true-to-life PET-associated internalization and mitochondrial dysfunction in lung-relevant models

Gabriel Ferraz,[1,2] Gustavo Bitencort,[1] Laia Pareras,[2] Santi Trischitta,[2,3] Javier Gutiérrez,[2] Alba Hernández,[2] Laura Rubio,[2] Roberta Urban[1*]

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Airborne micro and nanoplastics (MNPs) are emerging inhalation hazards, yet their occurrence in school environments and associated biological effects remain poorly understood.[1] This study combined the environmental characterization of atmospheric MNPs in a Brazilian elementary school[2] with a preliminary toxicological evaluation of a representative true-to-life polyethylene terephthalate (PET)[3] material in lung-relevant in vitro models. Atmospheric MNPs were detected indoors and outdoors, ranging from LOD to 60.16 items m^{-2} day^{-1} indoors and from LOD to 168.03 items m^{-2} day^{-1} outdoors. Particles were predominantly fragments, and μ-Raman analysis identified polyester as the major component, with ethylene vinyl acetate (EVA), polyethylene (PE), and PET also detected (**Figure 1**).

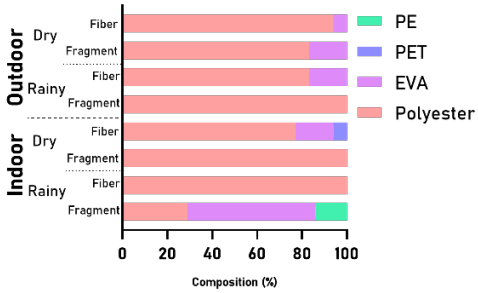

Fig. 1. Polymer composition of atmospheric microplastics and nanoplastics collected in indoor and outdoor environments of a Brazilian elementary school.

To investigate PET-associated cellular responses in lung-relevant systems, differentiated THP-1 (dTHP-1) cells and a Calu-3/dTHP-1 co-culture barrier model were exposed to a representative true-to-life PET material for 24 h. Qualitative confocal microscopy showed PET-associated signal in dTHP-1 cells and in the co-culture, while orthogonal views supported particle-associated localization in both macrophage-like and epithelial compartments (**Figure 2**).

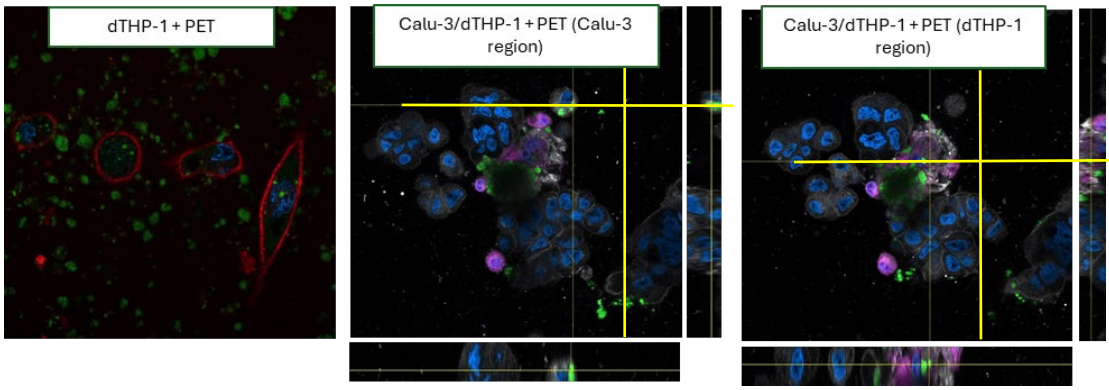

Fig. 2. Confocal images of dTHP-1 and Calu-3/dTHP-1 co-culture after 24 h exposure to PET. Cell membrane, white; nuclei, blue; dTHP-1 cytoplasm, magenta; PET-associated iDye signal, green

Mitochondrial effects were then assessed in the Calu-3/dTHP-1 co-culture after exposure to 2.5, 10, and 20 μg cm^{-2} PET using Mitoprobe™ assay. One-way ANOVA followed by Dunnett's multiple comparisons test ($\alpha = 0.05$) showed no significant effect at 2.5 μg cm^{-2} ($p = 0.0730$), but significant reductions in the high-fluorescent population at 10 μg cm^{-2} ($p = 0.0020$) and 20 μg cm^{-2} ($p = 0.0040$), consistent with loss of mitochondrial membrane potential. Together, these findings link a real-world school exposure scenario to early PET-associated cellular responses in a lung barrier-relevant model.

Acknowledgements: São Paulo Research Foundation (FAPESP) grants 2022/03087-9, 2023/06768-0 and 2025/11879-0. **References**: [1]Zhang et al.; *Earth Sci Rev* **2020**, 103118.; [2]Ferraz et al.; *Chemosphere* **2024**, v. 369, p. 143886. [3] Villacorta et al.; *J. Hazard. Mater* **2022**, v. 439, p. 129593.

EES - D4 - P28
Optimising reaction efficiency with surfactants

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[1]School of Chemistry, University of Leeds, UK; [2]School of Mechanical Engineering, University of Leeds, UK; [3]Chemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, UK.

Modern organic chemistry relies heavily on petroleum-based organic solvents, creating significant environmental burdens. Surfactants in water can be utilised to replace organic solvents and facilitate greener routes to organic molecules.[1] While expensive designer surfactants, such as TPGS-750-M and PS-750-M, are principally used, inexpensive and commercially available surfactants can perform equally well, making a process economically viable for large–scale industrial applications. The ***surfactant_map***[2] is a data-driven tool developed within the Institute of Process Research and Development (iPRD) at the University of Leeds, to guide rational surfactant selection for any given reaction.

A major barrier to the broader adoption of surfactant-enabled reactions lies in reaction work-up/purification. The amphiphilic nature of surfactants makes their removal particularly challenging, often requiring large volumes of organic solvents during work-up, negating the sustainability benefits of these reactions. A coalescing separator is a depth filter made from meltblown media that utilises both surface and gravity forces to separate immiscible liquids.[3,4] Coalescing filters are effective at breaking strong emulsions, making them well suited for overcoming the challenges associated with surfactants at the work-up/purification stage. This work has demonstrated the successful application of a novel coalescing separator, developed within the iPRD, to effectively eliminate surfactant contamination for high-yielding surfactant-enabled S_NAr and amide coupling reactions, previously optimised using the ***surfactant_map.*** Furthermore, the coalescing separator can be integrated into a continuous platform, offering the potential for continuous surfactant-enabled synthesis with in-line extraction and surfactant recycling.

Overall, the implementation of the ***surfactant_map,*** continuous flow chemistry and coalescing separators to deliver cost-effective, high-yielding surfactant-enabled reactions free from surfactant contamination represents a significant step toward industrially relevant, low-waste aqueous reaction platforms.

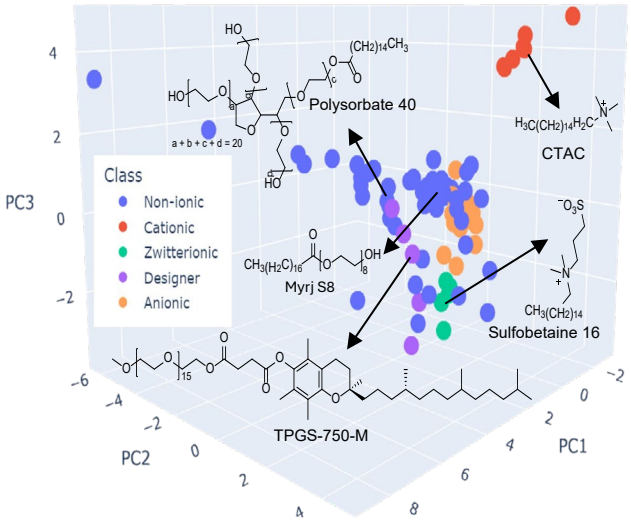

Fig. 1. The ***surfactant_map***.[2]

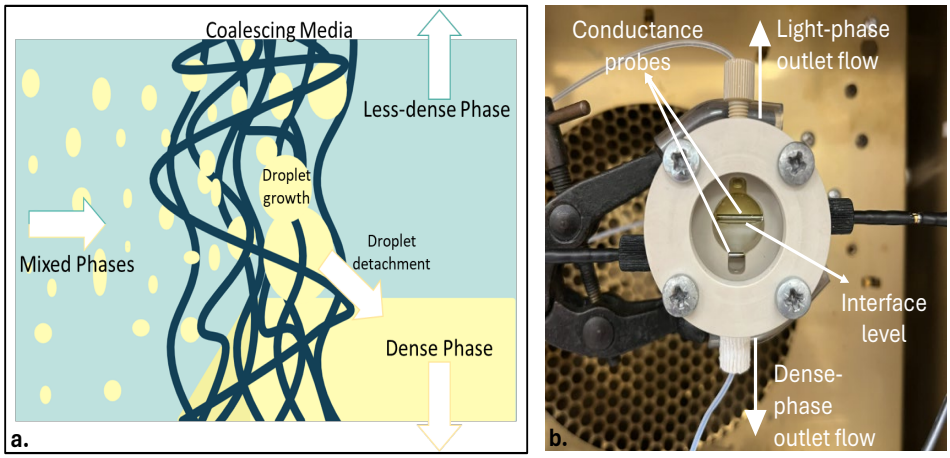

Fig. 2. **a.** Schematic of phase separation with a coalescing filter. **b.** Front-on view of the coalescing separator.

[1]B. Lipshutz et al., *Green Chem.,* **2024**, *26*, 739-752.
[2]K. Sharma et al., *Chem. Sci.,* **2024**, *15*, 5764-5774.
[3]J. Daglish et al., *OPRD,* **2024**, *28*, 1979-1989.
[4]B. Rowley et al., *React. Chem. Eng.*, **2025**, *10*, 392-397.

EES - D4 - P29

Revealing the extraction and coordination behavior of novel cyclohexyl o-oxydiamides ligand toward Pu(IV) μ

Qi Chen, Taihong Yan, Tianchi Li, Yandong Sun, Ye Zhang, Xiao Ge.
China Institute of Atomic Energy

Plutonium is of strategic importance. The study of Pu selective separation from nuclear industry liquid waste is crucial for Pu recovery. The present study is based on the plutonium-selective specific ligand o-phenoxydiamide, the benzene ring in its structure was replaced by cyclohexane, and the new cyclohexyl o-oxydiamide (R-CAD) was predicted to have a spatial spin while maintaining a high charge density, will be involved in the coordination with Pu(IV) as a tetradentate ligand, and will facilitate for Pu(IV) extraction. The coordination behavior was further explored by slope analysis, Ultraviolet-Visible titration, and FT-IR analysis, which proved that R-CDAforms of 1:1 and 1:2 metal/ligand complexing with Pu(IV) through four hard oxygen (ether oxygen and carbonyl oxygen) in the structure, with the 1:2 complexes displaying higher stability. Density functional theory (DFT) calculations revealed that the carbonyl oxygen atom in the complex had a far greater affinity for Pu(IV) than did the ether oxygen atom. In addition, the 1:2 metal/ligand complex single-crystal structure formed by R-CDA with Pu(IV) has been discovered for the first time in a breakthrough manner, and the coordination form has been elucidated intuitively. On the other hand, it was confirmed that R-CDA has good acid and irradiation stability. The present study not only enriches the theoretical knowledge of the coordination chemistry of Pu(IV) but also offers fresh perspectives on the design of separation ligands for plutonium in the nuclear industry.

The Continuous-Support Basic Scientific Research Project (BJ22002903) and provided funding for this research.

[1]Chen, Q.; Li, B.; Wang, J.; Zhu, H.; Chen, X.; Hu, Y.; Zhou, J.; Wang, W.; Zheng, W.; Yan, T. Selective Coordination Behaviors of Uranium(VI) with Novel Asymmetrical Tetra-alkylcarbamides. *Journal of Molecular Liquids*. **2023**, 371, 120924. DOI: 10.1016/j.molliq.2022.120924.
[2]Chen, Q.; Liu, Y.; Li, Z.; Li, B.; Wang, C.; Wang, J.; Hu, Y.; Wang, W.; Shi, W.; Yan, T. Unfolding the Extraction and Coordination Behaviors of Trivalent Lanthanides by two Novel Cyclohexyl O-oxydiamides Ligands. *Separation and Purification Technology*. **2023**, 318, 123876. DOI: 10.1016/j.seppur.2023.123876.

EES - D4 - P30

Selective extraction of plutonium(IV) by novel diphenylpyridine diamide extractants

Yao Liu, Junli Wang, Wang Junli, Le Yuhang, Wang Hui, Wang Wentao, Li Baole, Ye Guoan, Yan Taihong
China Institute of Atomic Energy

Three novel diphenylpyridine diamide extractants, PPDA, PDBA and PMDA, were designed and synthesized for the selective extraction of Pu(IV) from complex nitric acid systems. Their extraction behavior was systematically investigated by solvent extraction experiments, spectroscopic titrations and density functional theory calculations. All three ligands exhibited excellent extraction ability toward Pu(IV) and high selectivity over competing actinides and fission products. In particular, they enabled effective separation of Pu(IV) from other tetravalent metal ions, which remains a major challenge in plutonium separation chemistry. Slope analysis and UV–Vis titration showed that the extracted complexes had a 1:1 metal-to-ligand stoichiometry. Thermodynamic studies indicated that the extraction process was spontaneous and exothermic under ambient conditions. The stability constants further confirmed the strong complexation ability of these ligands toward Pu(IV). DFT calculations revealed that the stronger Pu–O interaction, compared with other metal–oxygen bonds, plays a key role in the observed selectivity. In addition, the ligands showed good reusability and irradiation stability, maintaining their extraction performance after repeated cycles and gamma irradiation. These results demonstrate that the newly developed diphenylpyridine diamide ligands are promising candidates for the efficient and selective separation of Pu(IV) from complex systems.

Supported by basic support for stability of China Institute of Atomic Energy (BJ030261224901).

[1]Liu, Y.; Wang, J.; Le, Y.; Wang, H.; Wang, W.; Li, B.; Ye, G.; Yan, T. Selective extraction of plutonium(IV) by novel diphenylpyridine diamide extractants from complex system: An experimental and theoretical study. *Separation and Purification Technology.* **2025**, 379, 134590.
[2]Liu, Y.; Wang, J.; Le, Y.; Wang, H.; Wang, W.; Li, B.; Yan, T. Highly selective separation of tetravalent plutonium from complex system with novel phenylpyridine diamide ligands. *RSC Adv.*, **2024**, 14, 560–567

EES - D4 - P31
A green and efficient aqueous LLPS platform for metal ion separation

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The traditional aqueous-organic biphasic extraction for separating metal ions faces major challenges due to heavy reliance on volatile organic solvents and the resulting refractory radioactive waste. Aqueous liquid-liquid phase separation (LLPS) offers an alternative by forming a condensed separation phase directly in water, yet its research in metal ions separation is still limited. Here, we establish LLPS as a separation platform through two complementary modes: self-extracting and extractant-loaded. In the self-extracting mode, quaternary ammonium surfactants/HFIP condensed phase enables near-quantitative extraction of Au(III), Pt(IV), and Pd(II) under mild aqueous conditions. This mode also maintains selective Au(III) recovery from real PCB leachates at an extreme Cu/Au mass ratio of 4300:1, with an enrichment factor of 25. Moreover, using only 1 mM thiourea as the stripping reagent, the condensed phase sustains five extraction-stripping cycles with average extraction and stripping yields of 97.6% and 97.9%, respectively. In the extractant-loaded mode, an SDS/CTAB/HFIP condensed phase encapsulates commercial extractants to provide programmable radioactive-ion separation. In simulated high-level liquid waste, the extractant-loaded aqueous LLPS system achieved a U(VI) distribution ratio of 1.29×10^3, with separation factors exceeding 10^3 over coexisting lanthanides and alkaline-earth metal ions, demonstrating highly selective U(VI) partitioning. After stripping with 0.05 M EDTA, this system maintains extraction yields above 98% over five cycles, while the average stripping yield remained above 92%. Despite their distinct target chemistries, both modes follow the same design logic: LLPS forms a small and independent condensed phase in the original aqueous phase. Selective metal ions partitioning is governed by the synergistic effect of supramolecular interactions, particularly electrostatic and hydrophobic interactions, and metal-ligand coordination. Above all, these results show that aqueous LLPS is a tunable, green and efficient framework for selective metal-ion separation across distinct separation scenarios.

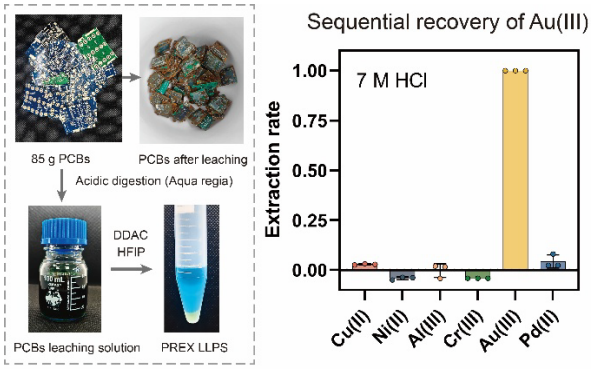

Fig. 1. Practical application for PMs separation from discarded mobile phone PCBs.

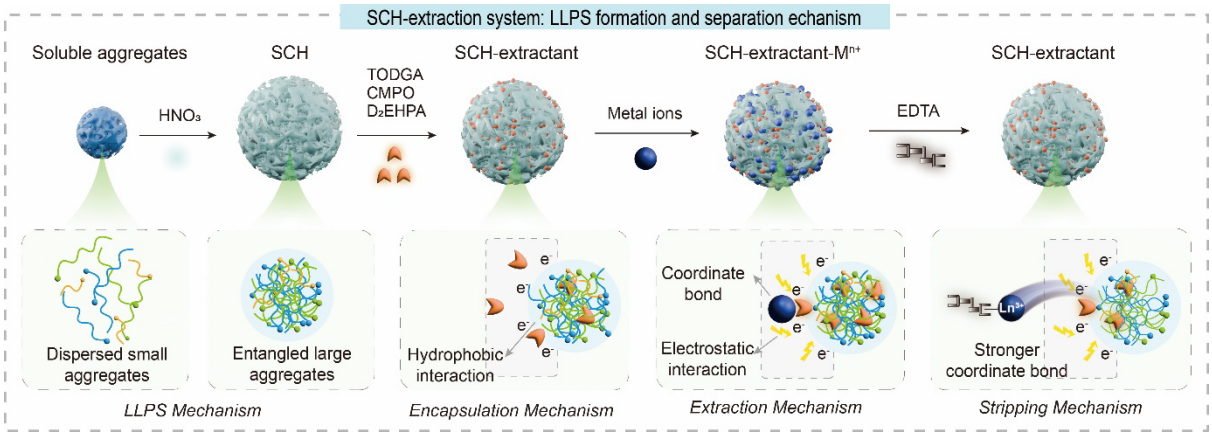

Fig. 2. Schematic of the extractant-loaded system (SCH-extraction system) formation process and generation mechanism.

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[1]Yan, R.; Wang, W.; Wang, J.; Cao, Z.; Fang, S.; Ye, G.; Yan, T. *Chem. Eng. J.* **2026**, 529, 173090.
[2]Yan, R.; Hu, Y.; Wang, W.; Cao, Z.; Cao, M.; Zheng, W.; Ye, G.; Yan, T. *Adv. Sci.* **2026**, DOI: 10.1002/advs.75493.

EES - D4 - P32
Green extractive desalination with designer green solvents for freshwater production

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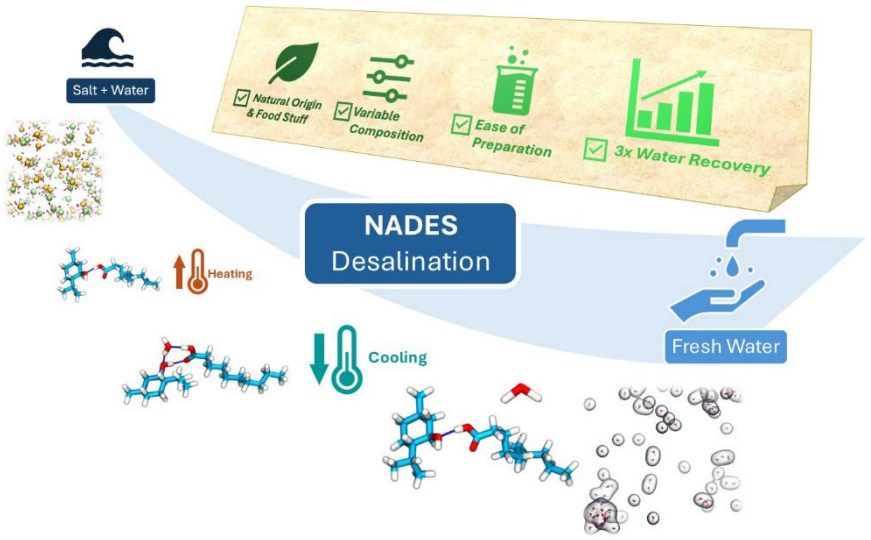
Extractive desalination represents an affordable, membrane-less approach to desalinate water, which can operate solely using low-temperature waste heat from industrial sources. It has been suggested as a viable alternative for producing freshwater from saline sources by employing long-chain carboxylic acids.[1] To enhance the freshwater yield, ionic liquids (ILs)[2-3] and amines[4] have been explored as replacements for carboxylic acids. Nevertheless, amines exhibit significant toxicity, and ILs frequently contain hazardous elements, particularly the bis(trifluoromethanesulfonyl)imide anion.
To balance high water recovery with a green and food-based solvent selection, we identified the most effective designer green solvent for extractive desalination, especially the hydrophobic natural deep eutectic solvent (NADESs). Initial findings show that these NADESs improve overall freshwater yield and salt rejection relative to their individual constituents. This enhancement occurs through the disruption of robust dimeric hydrogen bonds between solvent molecules, which otherwise impede water uptake, and by extending the duration of hydrogen bonds formed between the extractant and water. The resulting fresh water exhibits minimal salinity, complying with World Health Organization guidelines, and is suitable for direct consumption by humans and land animals—in contrast to earlier proposed extractants.



[1]A. Bajpayee, T. Luo, A. Muto and G. Chen, Energy & Environ. Sci., **2011**, 4, 1672.
[2]O. K. Choi, H. C. Lim, Y. Cho, A. E. Cho, A. A. Hasan, G. P. Lithoxoos, H. A. Aljama, S.-H. Choi, Y. C. Choi and J. W. Lee, Desalination, 2023, 557, 116608–116608.
[3]G. M. Durling, T. Milazzo, E. Marin-Rimoldi, J. A. Ouimet, W. A. Phillip, E. J. Maginn, T. Luo and B. L. Ashfeld, Journal of the American Chemical Society, 2025, 147, 20294–2030
[5]O. K. Choi, J. H. Seo, G. S. Kim, Z. Hendren, G. D. Kim, D. Kim and J. W. Lee, J. Hazard. Mater., 2021, 403, 123636.

EES - D4 - P33

MXene-promoted Ni-based bimetallic catalysts on CeO_2–ZrO_2 for efficient hydrogen production via steam methane reforming

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Hydrogen is widely recognized as a key energy carrier in the global transition toward low-carbon and sustainable energy systems, with applications across industrial processes, power generation, and transportation. Among available technologies, steam methane reforming (SMR) remains the most cost-effective and industrially established route for large-scale hydrogen production. However, conventional SMR catalysts are limited by sintering, coke formation, thermal instability, and reduced activity at lower operating temperatures, highlighting the need for advanced and durable catalyst systems. Herein, we report the development of multifunctional SMR catalysts based on MXene-promoted Ni–Co bimetallic nanoparticles supported on CeO_2–ZrO_2. The optimized catalyst composition consists of Ni, Co, and MXenes dispersed on CeO_2–ZrO_2 support. This integrated design combines the high oxygen storage capacity and thermal stability of the CeO_2–ZrO_2 support with the synergistic effects of Ni–Co bimetallic active sites and MXene promotion. This results in enhanced metal dispersion, strengthened metal–support interactions, and improved resistance to sintering and carbon deposition. The catalysts were comprehensively characterized using X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), dynamic light scattering (DLS), thermogravimetric analysis (TGA), and Brunauer–Emmett–Teller (BET) surface area analysis. Structural characterization confirmed a high surface area and uniform distribution of active sites. Catalytic performance evaluation demonstrated high methane conversion and enhanced hydrogen yields (>90%) under SMR conditions. Overall, this multifunctional catalyst strategy effectively addresses the limitations of conventional SMR catalysts, offering a promising pathway toward more efficient and sustainable hydrogen production.

Acknowledgement: The authors acknowledge financial support provided by King Fahd University of Petroleum and Minerals (KFUPM), Kingdom of Saudi Arabia, for this research under the IRC-HTCM Project (INHT2525).

EES - D4 - P34
Natural Algerian diatomite as a low-cost adsorbent for Bezacryl yellow dye removal

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Water pollution by synthetic dyes is a significant environmental issue in Algeria. This study evaluates Algerian diatomite known Kieselguhrs as a low-cost and sustainable adsorbent for the removal of Bezacryl Yellow (BY) from aqueous solutions. Diatomite (D) is characterized by different physical-chemical methods (X-ray diffraction, scanning electron microscopy, Fourier transform infrared and Thermogravimetric analysis (TGA). The adsorbent exhibits a specific surface area of 163 $m^2.g^{-1}$, determined by the Sears method[1,2]. Batch adsorption experiments were conducted under various conditions of pH, adsorbent dosage, dye concentration, contact time, and temperature. Adsorption was found to be strongly favored in highly alkaline media at pH =12, B Yremoval rate increases as pH increases. Adsorption equilibrium is reached after 20 mins of contact time. Kinetic data were best described by the pseudo-second-order (PSO) model, while equilibrium results followed the Temkin isotherm, indicating uniform adsorption energy distribution. A maximum adsorption capacity of 212 mg.g-1 was obtained. Thermodynamic analysis revealed a negative enthalpy change ($\Delta H° = -9.451$ kJ mol^{-1}), confirming an exothermic process favored at lower temperatures. These results demonstrate that Algerian diatomite is an efficient, eco-friendly, and economically viable adsorbent for the removal of Bezacryl Yellow from contaminated water.

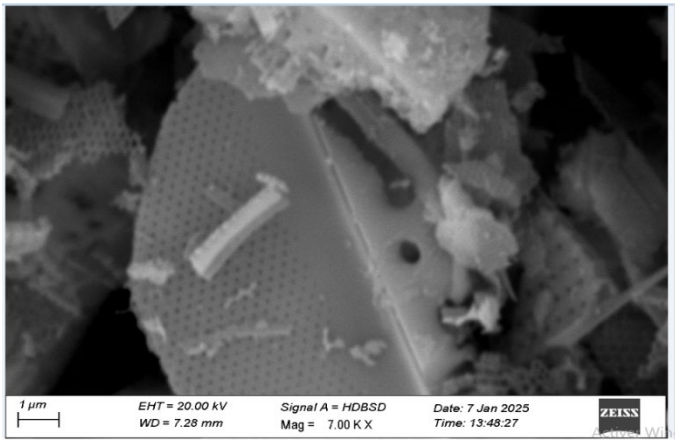

Fig. 1. SEM micrograph of raw diatomite powder at scale bar of 1 µm.

[1] Sears,G W . Anal. Chem. 1956, 28; 1981
[2] Bhattacharyya K G.; Sen Gupta S. J Colloid Interface Sci. 2007, 310, 411–424

EES - D4 - P35

Enhanced photocatalytic hydrogen evolution via broad visible-light harvesting in g-C_3N_4/polymer heterostructures

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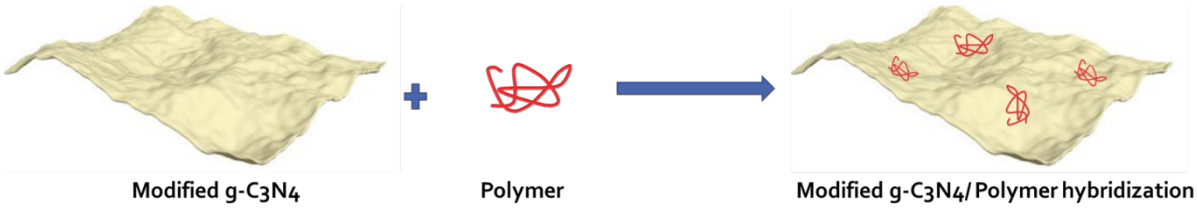
Graphitic carbon nitride (g-C_3N_4) is a widely investigated metal-free polymeric semiconductor for photocatalytic hydrogen evolution and CO_2 reduction because of its suitable band gap (2.7 eV), visible-light activity, thermal stability, low cost, and non-toxic nature[1]. However, its practical photocatalytic performance remains limited by rapid charge-carrier recombination and weak light absorption beyond 460 nm. To overcome these drawbacks, heterostructured photocatalysts based on g-C_3N_4 and organic conjugated polymers have attracted growing attention, owing to their tunable electronic structures and improved charge-transfer properties. In this work, modified g-C_3N_4 was hybridized with a conjugated polymer possessing broad visible-light absorption and good solubility to strengthen interfacial interactions and extend optical absorption, thereby enhancing photocatalytic activity. Among the prepared g-C_3N_4/polymer heterostructures, the g-C_3N_4/PFTBTA photocatalyst exhibited the best hydrogen evolution rate of 833.81 umol h^{-1} in the presence of ascorbic acid as a sacrificial agent. Notably, the g-C_3N_4/PFTBTA heterostructure delivered an outstanding apparent quantum yield (AQY) of 84% at 500 nm, outperforming all comparable materials reported to date.



The authors acknowledge the Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM) at King Fahd University of Petroleum and Minerals (KFUPM) for its support

[1]Mahmoud Kamal Hussien.,,. *Chemical Engineering Journal*. **2022**, *430*, 132853.

EES - D4 - P36

Energy-efficient and sustainable water desalination using flow electrode deionization with enhanced charge and ion transfer

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The increasing demand for freshwater requires the development of energy-efficient and sustainable desalination technologies. Flow electrode deionization (FEDI) is a promising electrochemical approach for continuous desalination; however, its performance is often limited by inefficient charge transfer and restricted ion transport within the system.
In this study, an enhanced FEDI system was developed by integrating a three-dimensional carbon foam current collector with ion exchange resin to enhance overall electrochemical performance. The carbon foam provides a highly conductive porous structure that enhances electron transfer, while the ion exchange resin facilitates ion migration by forming conductive pathways and reducing mass transfer resistance.
The optimized system achieved an average salt removal rate of 845 $\mu g \cdot cm^{-2} \cdot min^{-1}$ with a low electrical energy consumption of 1.64 $J \cdot mg^{-1}$, demonstrating energy-efficient desalination while maintaining competitive removal performance. This performance is attributed to reduced internal resistance and more efficient utilization of electrical charge.
These results demonstrate a practical strategy for improving electrochemical desalination systems and support the development of scalable, energy-efficient technologies for sustainable water treatment.

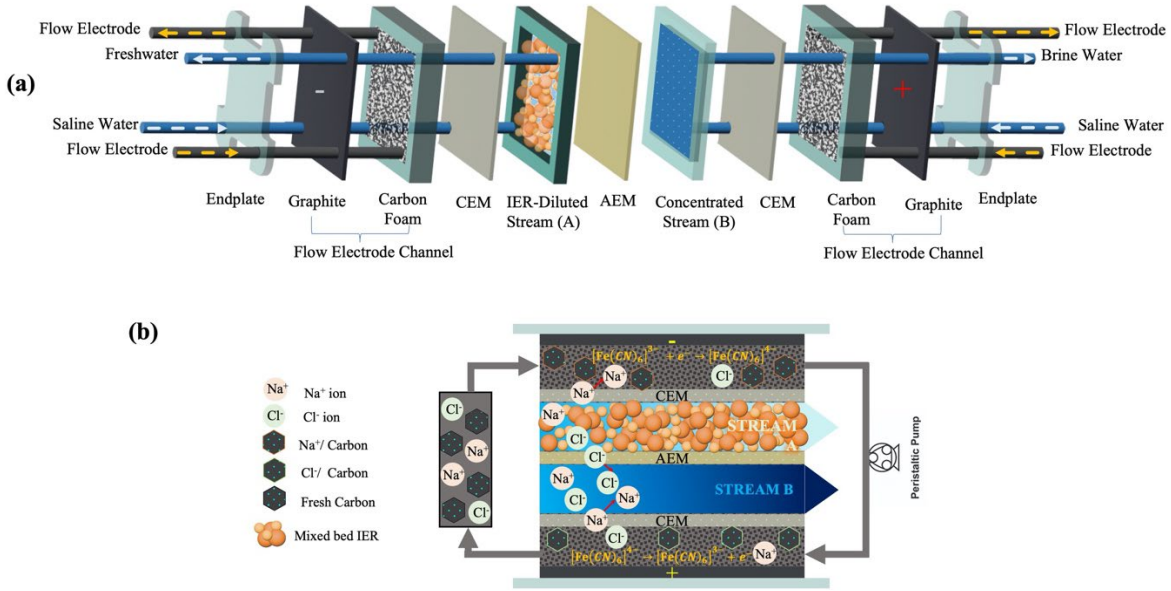

Fig. 3. (a) Schematic illustration of the flow electrode deionization (FEDI) system and (b) experimental setup used for continuous desalination.

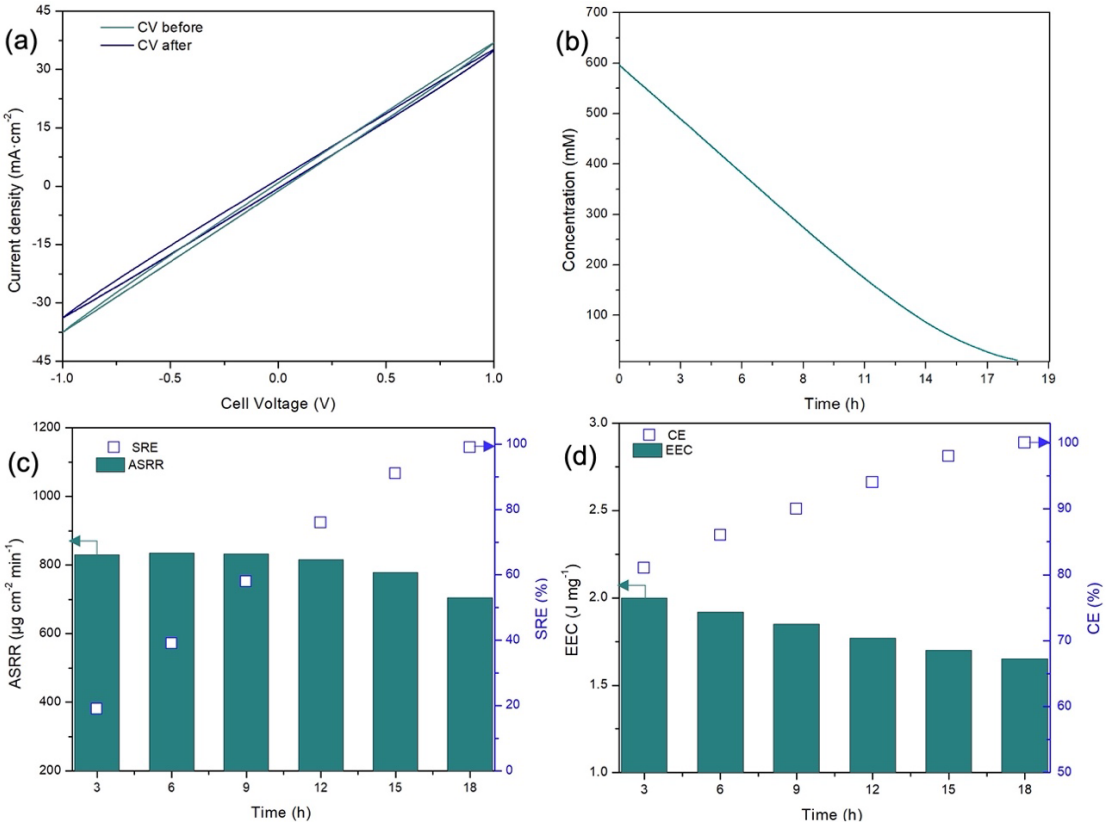

Fig. 2. Electrochemical and desalination performance of the optimized FEDI system: (a) cyclic voltammetry response, (b) salt concentration profile, and (c–d) key performance metrics including salt removal rate and energy consumption.

EES - D4 - P37
Graphene quantum dot-based nanostructured electrodes for advanced sodium ion batteries

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Tungsten disulfide (WS_2) is a layered transition metal dichalcogenide (TMD) with rich redox chemistry and a high theoretical capacity. It is therefore a promising anode material for sodium-ion batteries (SIBs). However, WS_2 suffers from low conductivity, structural instability upon cycling and limited sodium ion diffusion kinetics. The addition of nitrogen-doped graphene quantum dots (N-GQDs) to WS_2 can mitigate these issues. GQDs provide further active sites, an increased surface area, and can act as a structure regulator. Furthermore, the nitrogen doping of the GQDs provides a greater number of ion diffusion channels and leads to a higher charge carrier density.

N-GQDs with highly controllable bandgaps were first synthesised. The edge shapes and size of the nanoparticles were selected, alongside the battery electrolyte pH, to provide the most beneficial properties for SIBs. Self-assembled low crystallinity tungsten disulfide nanosheets with embedded N-GQDs were grown on the surface of nickel foam via electrodeposition, creating a binder-free anode. SEM images confirmed the presence of the nanosheets, while EDX, UV Vis and Raman confirmed their composition. XRD and SAED data demonstrated that the interlayer spacing of the WS_2 was widened by 0.1 nm (from 0.62 to 0.72 nm) upon N-GQD addition.

The widened interlayer spacing facilitates sodium-ion intercalation and conversion recations. The N-GQD/ WS_2 electrode has a specific capacity of 311 mAh/ g at 1 A/ g, compared to 206 mAh/ g for the electrode without N-GQDs integrated.

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Innovative Materials (IM)

IM - D4 - P01

Enhancing the flame retardant performance of expandable polystyrene using halogen-free additives and synergists

Pinar Ozmen[1,2], Hayal Bulbul Sonmez[2]
[1]CFN Kimya Inc., Turkiye; [2]Gebze Technical University, Turkiye

The primary objective of this study is to synthesize and characterize expandable polystyrene (EPS) containing halogen-free flame retardant additives, and to evaluate its flame retardancy performance together with other critical properties, including mechanical strength, thermal stability, particle size distribution, and homogeneity. To accomplish this objective in a systematic and controlled manner, various halogen-free flame retardants with different functional groups are incorporated into the EPS synthesis process. This project aims to analyze the effects of flame retardants on flammability resistance, as well as monitoring their influence on the overall performance of the final EPS product. Special attention is given to ensuring that improvements in flame retardancy do not compromise the essential properties of EPS. Through systematic formulation development and optimization, the present research seeks to create a balanced material that exhibits enhanced fire resistance alongside optimized physical, mechanical, and thermal characteristics. This research contributes to the advancement of flame-retardant materials by providing a comprehensive understanding of how halogen-free flame retardants affect the synthesis and performance of EPS, thereby supporting safer and more sustainable applications across various industries.

IM - D4 - P02

Two salt-surfactant mesophases: Synthesis of mesoporous MgM_2O_4 (M=Mn, Fe and Co) electrodes and their electrochemical properties

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Mesoporous magnesium metal oxides or MgM_2O_4 (M=Mn (II), Fe (III) and Co (II)) have been synthesized by using transition metal nitrate salts including ([Mn $(H_2O)_4(NO_3)_2$], Co $(H_2O)_6(NO_3)_2$, and [Fe $(H_2O)_9(NO_3)_3$]), two surfactants; hexadecyltrimethylammonium bromide (CTAB), oligo (ethylene oxide) in water and ethanol as a solvent. This method of synthesis is called the molten salt-assisted self-assembly method (MASA), and The resulted clear solutions of the two salt-surfactant systems are lyotropic liquid crystalline phase (LLC) or mesophase features. The liquid crystal solutions and mesophases are analyzed using ATR-FTIR, XRD, and POM instruments. ATR-FTIR spectra for both salt surfactant samples show distinct features at 3600-3000 and 1650-1600cm^{-1}, which are related to stretching and bending modes of water species, respectively, as well as 1500-1290cm^{-1} due belongs to nitrate species. Low-angle XRD patterns show the ordered structure of LLC mesophases. The solutions are drop-cast coated over a glass substrate, calcined at elevated temperatures, and analyzed through high-angle XRD patterns. The crystallization starts even at 300 °C, and by calcination up to 700 °C, the corresponding mesoporous magnesium metal oxides are obtained. The porosity of the magnesium metal oxides is analyzed through XPS, and SEM.

Further, to investigate the catalytic performance of the samples in water oxidation, they are coated onto fluorine-doped tin oxide (FTO) substrates and subsequently calcined to obtain porous electrodes. These electrodes are then studied for their electrochemical properties using cyclic voltammetry (CV), and multi-step chronopotentiometry and amperometry (MCP-MCA) measurements. The results indicate that cobalt-based mesoporous electrodes have higher stability compared to manganese and iron-based electrodes, and exhibit small Tafel slope values in the range of 39–46 mV dec^{-1}, indicative of favorable reaction kinetics for water oxidation. The stability and electrochemical performance of those magnesium metal oxides are going to be tested over a graphite (GR) substrate.

[1]Raza, H. A.; Karakaya, I.; Dag, Ö. Nanoarchitectonics of Mesoporous Cafe2O4 Thin-Film Electrodes from Salt-Surfactant Lyotropic Liquid Crystalline Mesophases and Their OER Performance. *ACS Applied Energy Materials* **2023**, *6* (18), 9681–9697. DOI:10.1021/acsaem.3c01776.

IM - D4 - P03

Calcone–schiff base hybride coated titanium surfaces with light-induced antibacterial activity

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Chalcone-based compounds incorporating a Schiff base hybride have attracted considerable interest due to their extended π-conjugation and versatile structural framework. Combining the chalcone (α,β-unsaturated carbonyl) and imine (–C=N–) functionalities enhances electronic delocalisation, resulting in enhanced optical, thermal and mesomorphic properties. These hybrid systems have been widely investigated for potential applications in nonlinear optics and liquid crystalline materials, as well as in bioactive agents with antibacterial, anticancer and antioxidant properties [1].

In this study newly synthesized chalcone schiff base hybride compound was coated onto titanium surfaces using the drop-casting method with a dimethylformamide (DMF) solution [2]. Following coating, XRD, SEM, EDX, FTIR and contact angle measurement tests were performed. The phthalocyanine-coated surfaces exhibited greater hydrophobicity than the uncoated surfaces. Activity tests against E. coli and S. aureus bacteria were then performed on the coated surfaces under both dark and daylight conditions.

Keywords: Chalcone, Schıff base, Titanium, antibacterial surface.

This work was supported by Karadeniz Technical University, Trabzon (Project Number:16509).

[1]Emirdağ S, Ulusoy NG, Kahriman N, Serdaroglu V, Türkmenoglu B, Yayli N. J. Mol. Struct. 2025, 1345, 143101.

[2]Durdu S, Sivlin D, Ozcan K, Kalkan S, Keleş O, Usta M, Surface characterization and antibacterial efficiency of well-ordered TiO2 nanotube surfaces fabricated on titanium foams Sci. Rep. 2024, 14, 618.

IM - D4 - P04

Impact of PZA Incorporation on the thermal stability, carbon yield, and electrical conductivity of 3D-printed polymer-derived carbons

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This work investigates the thermal stability, carbonization behavior, and electrical performance of photopolymer-derived carbons obtained from resins containing different proportions of pyrazinamide (PZA) as a partial substitute for divinylbenzene (DVB). Among the PZA–DVB series, particular attention was given to samples MDVB (0% PZA) and MPZA (100% PZA), which represent the two compositional extremes and therefore enable elucidation of the structural effects induced by PZA incorporation on the properties of the resulting pyrolytic carbon. Both materials were fabricated via vat photopolymerization followed by thermal pre-oxidation at 300°C and pyrolysis at 900°C under nitrogen, following similar methods than those previously published [1-2]. Mass yield measurements revealed a strong dependence on PZA content: while MDVB retained 20.0% of its mass after pyrolysis, MPZA exhibited a markedly lower final yield of 5.7%, indicating extensive volatilization and structural fragmentation in the PZA-rich resin. Consistent with this trend, MPZA also displayed significantly higher volume shrinkage (~94%) compared to MDVB (~84%) (Figure 1.a-b), confirming that PZA alters the degradation pathway and reduces the char stability of the polymer network. Thermogravimetric analysis (TGA) further showed that the precursor MDVB oxidize at higher temperatures than MPZA (Figure 1.c), while both pyrolyzed materials exhibit the characteristic high thermal stability of carbonaceous solids under nitrogen atmosphere. Proximate and elemental analyses confirmed the substantial increase in fixed carbon content after pyrolysis (MDVB: 93.8%; MPZA: 82.9%), along with a drastic reduction in H/C ratios, indicative of extensive aromatization. Nitrogen incorporation was higher in the PZA-rich sample (Figure 1.d), validating PZA as an efficient nitrogen source. Electrical conductivity measurements revealed that MPZA achieves significantly higher conductivity (~1037 S/m) than MDVB (~155 S/m). These results demonstrate that PZA strongly influences carbon yield, nitrogen incorporation, microstructural evolution, and electrical performance in polymer-derived 3D carbon architectures.

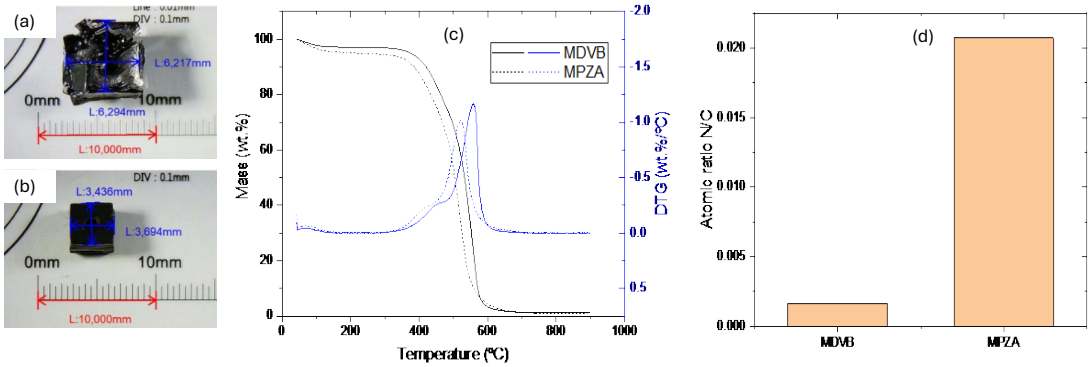

Fig. 1. Photographs of (a) sample MDVB and (b) sample MPZA, (c) TGA and (d) atomic ratios N/C obtained by elemental analysis.

Acknowledgements: The authors would like to express their sincere gratitude to the DACIU Program (*Desarrollo de las Altas Capacidades Intelectuales en la Universidad*) of Fundación Avanza for its support. Noelia Corrochano Guijarro and Jose L. Diaz De Tuesta acknowledge financial support through the grant 2022-T1/AMB-23946 funded by *Comunidad de Madrid*. Jose L. Diaz De Tuesta also acknowledges the financial support through the grant CNS2024-154264 funded by *Agencia Estatal de Investigación*.

[1]Silva, A. S.; Diaz de Tuesta, J. L.; Henrique, A.; Roman, F. F.; Omralinov, D.; Steldinger, H.; Gläsel, J.; Etzold, B. J. M.; Silva, J. A. C.; Silva, A. M. T.; Pereira, A. I.; Gomes, H. T. *Chem. Eng. J.* **2024**, *499*, 156574.
[2]Henrique, A.; Steldinger, H.; Diaz de Tuesta, J. L.; Gläsel, J.; Rodrigues, A. E.; Gomes, H. T.; Etzold, B. J. M.; Silva, J. A. C. *Chem. Eng. J.* **2023**, *472*, 145138.

IM - D4 - P05
3D printing of nanocomposites-some assembly required

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Using just a handful of raw material building blocks, nature has succeeded in using different design and fabrication strategies to yield a broad canvas of hierarchical structures. To date, the generation of synthetic photonic materials has followed two diverse routes which have made considerable progress in separately delivering intrinsically and extrinsically ordered materials. Intrinsically photonic materials have been achieved through self-assembly protocols, such as evaporation-induced self-assembly, shear alignment, and application of magnetic field. Attention in this field has also been garnered by renewable biopolymers such as guanine, cellulose nanocrystals, hydroxypropyl cellulose.[1-4] Extrinsic structuring for the generation of photonic devices has focussed on techniques borrowed from micro-electro-mechanical systems (MEMS) technologies, such as e-beam lithography and wet chemical etching in silicon, glass, metals, diamond, and other high refractive-index dielectrics.
Creating responsive optical elements with multiple components requires a holistic approach which marries smart material development with cutting edge fabrication techniques to combine intrinsic and extrinsic structuring.[5,6]
Herein, this is realised through the combination of three elements: 1) two-photon polymerisation (2PP) for the generation of biomimetic structures with extrinsic order; 2) nanomaterial dispersions to alter the refractive index of hydrogels and achieve a photonic bandgap within the polymeric matrix and; 3) stimuli-responsive hydrogels that exhibit a controllable response under stimulation.

Fig. 1. Schematic of direct laser writing process in ordered photoresists. a) Polymerisation being achieved in a voxel-by-voxel manner. b) The effect of fabrication parameters on the assembled nanocomposite. c) Response of photonic arrays in response to chemical stimuli.

C.D. acknowledges funding from Research Ireland under the Pathway Programme (Grant No. 22/PATH-S/10790).

*1. Zhao, T. H.; Parker, R. M et al. Advanced Functional Materials **2019**, 29 (21), 1804531.*
*2. Chan, C. L. C.; Bay, M. M. et al. Advanced Materials **2019**, 31 (52), 1905151.*
*3. Parker, R. M.; Guidetti, G. et al. Advanced Materials **2018**, 30 (19), 1704477.*
*4. Berger, O.; Yoskovitz, E. et al. Advanced Materials **2016**, 28 (11), 2195-2200.*
*5. Qian, J.; Kolagatla, S. at al. Advanced Functional Materials **2023**, 33 (39), 2211735.*
*6. Faraone, T.; Qian, J. et al. Advanced Materials **2025**, 37 (43), 2504116.*

IM - D4 - P06
Silica-based degradable micromotors with potential environmental and health impact

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Degradable nanomaterials are increasingly recognized as a key enabler in tackling global sustainability challenges. Future material design must not only ensure safety and reduced ecological footprint, but also maintain, or ideally enhance, functional performance. Our research focuses on silica-based nanomaterials engineered with programmed degradability. Introducing controlled breakdown mechanisms significantly broadens their application scope, ranging from drug delivery systems and biomedical release platforms[1] to analytical technologies and environmental remediation strategies. To achieve this, we have integrated emerging degradable components, such as polyphosphazene segments, directly into the silica network. This approach has led to the development of advanced hybrid porous nanostructures that might combine on-demand functionality response with controlled tunable degradability (Figure 1).[2-5] Beyond static applications, we have extended these concepts to dynamic systems by designing silica-based micro/nanomotors. We demonstrated precise activation, deactivation, and directional control through a reversible external braking mechanism based on thermoresponsive bottle-brush polymers.[6-7] Despite these promising results, such complex motorized architectures require further investigation, particularly regarding navigation accuracy and controlled propulsion in biologically relevant microfluidic environments.

The Institute of Applied Chemistry acknowledges the funding for the project “Micromotors and nanomaterials for ecological applications” (DEGMOT) WST3 - F-5030820/028-2024

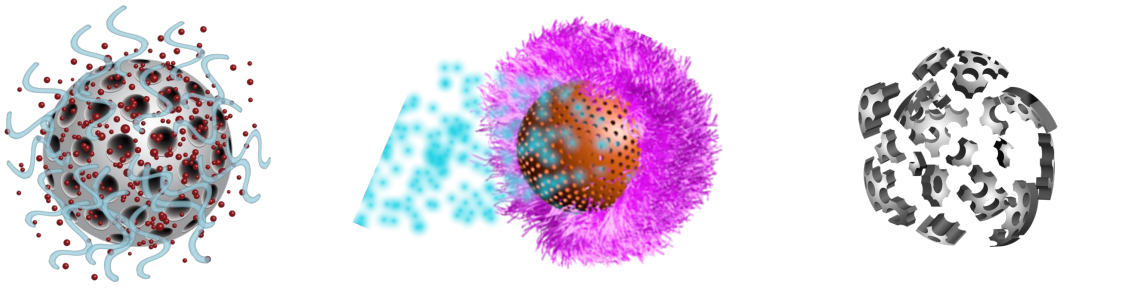

Fig. 1. Innovative micromaterials that safely break down after use, standing on three pillars

[1]Poscher, V.; Salinas, Y. Materials, **2020**, *13*, 3668–3691.
[2]Salinas, Y.; Hoerhager, C.; García-Fernández, A.; Resmini, M.; Sancenón, F.; Martínez Mánez, R.; Brüggemann, O.; *ACS Appl. Mater. Interfaces* **2018**, *10*, 34029−34038.
[3]Salinas, Y.; Brüggemann, O.; Monkowius, U.; Teasdale, I. *Nanomaterials* **2020**, *10*, 1030–1045.
[4]Poscher, V.; Teasdale, I.; Salinas, Y. *ACS Applied Nano Materials* **2019**, *2*, 655–660.
[5]Salinas, Y.; Poscher, V.; Brüggemann, O.; Teasdale, I. *Materials* **2022**, *15*, 4763.
[6]Salinas, Y.; Kneidinger, M.; Fornaguera, C.; Borrós, S.; Brüggemann, O.; Teasdale, I. *RSC Advances* **2020**, *10*, 27305–27314.
[7]Fiedler, C.; Ulbricht, C.; Truglas, T.; Wielend, D.; Groiss, H.; Brüggemann, O.; Teasdale, I.; Salinas, Y. *Chem. Eur. J.* **2021**, *27*, 1–7.

IM - D4 - P07

Efficient dissolution and selective recovery of gold from electronic waste using a recyclable ionic medium

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The significant socio-economic and technological importance of gold necessitates sustainable supply to meet the continuously rising demand. As the demand rises, recovering gold from secondary sources has become increasingly important, highlighting the need for environmentally and economically sustainable extraction processes.[1-5] In this study, gold was efficiently and rapidly leached quantitatively as Au(III) halometalate (Cl/Br) complexes and selectively recovered (~100%) in eight different hydrophobic ionic liquids (ILs) based on pyridinium, pyrrolidinium, and imidazolium at room temperature from both mixed metals solution and electronic waste (e-waste). ILs were recovered after extraction, and used for another two cycles for dissolution and recovery of gold thus demonstrating the economic sustainability of the developed process. Moreover, a techno-economic analysis of the method reveals attractive numbers for gold recovery, even without recycling of ILs. The background for the selective chemistry was studied comprehensively using diverse analytical techniques, complemented by density functional theory (DFT) calculations, and life cycle analysis (LCA). Furthermore, single crystal X-ray diffraction and DFT calculations revealed that non-covalent interactions between the cationic part of the IL and Au(III) halide are key for selective gold separation. The LCA study demonstrates that the process can lower CO_2 emissions by ~84.4% compared to conventional gold mining under the current Indian energy mix, with the potential for an almost complete emissions reduction (~99.9%) if powered by solar energy. The developed process is expected to pave the way for economic and environmentally sustainable recycling of multi-metals from e-waste.

Acknowledgements: A.N. and K.M.P. acknowledges the Marie Skłodowska-Curie Actions–European Commission post-doctoral grant (REWCHEM, Grant agreement ID: 101152892) and Sustain-a-Print project (Grant agreement ID: 101070556) from European Commission for research funding. P. B. acknowledges, Ramón y Cajal grant from Spanish State Investigation Agency (Grant no. J03416).

[1]Nag, A.; Islam, M. R.; Pradeep, T. *ACS Sustainable Chemistry & Engineering* **2021**, *9*, 2129-2135.
[2]Nag, A.; Singh, M. K.; Morrison, C. A.; Love, J. B. *Angew. Chem. Int. Ed.* **2023**, *62*, e202308356.
[3]Nag, A.; Morrison, C.; Love, J. *ChemSusChem* **2024**, *17*, e202301695.
[4]Nag, A.; Morrison, C. A.; Love, J. B. *ChemSusChem* **2022**, *15*, e202201285.
[5]Nag, A.; Qurashi, A.; Morrison, C. A.; Moth-Poulsen, K.; Pradeep, T.; Love, J. B. *Coord. Chem. Rev.* **2026**, *548*, 217186.

IM - D4 - P08
Magnetically induced drug release from doxorubicin-loaded niosome nanocarriers

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Niosomes is vesicular nanocarriers composed of nonionic surfactants and cholesterol which have emerged as versatile systems for controlled drug delivery due to their high biocompatibility, structural stability, and ability to encapsulate both hydrophilic and hydrophobic drugs.1,2 This study aims to design and evaluate a magnetically stimuli-responsive niosomal system for the control release of the anticancer drug doxorubicin under alternating magnetic field exposure. The formulation combined doxorubicin and magnetic nanoparticles loaded niosomes for controlled release cancer therapy. Dextran coated iron oxide magnetic nanoparticles were synthesized by a co-precipitation method under a nitrogen atmosphere3,4 and niosomes were synthesized by the thin-film hydration technique made of Span 60 and cholesterol.5 The loading efficiency of the doxorubicin was between 60–70%. The hydrodynamic diameter measured as the average number was found to be 188 ± 68, 141 ± 86 and 169 ± 69 nm for the plain niosomes, niosomes-doxorubicin and niosomes-doxorubicin-magnetic nanoparticles, respectively. The thermally mediated release of doxorubicin was monitored using fluorescence spectroscopy and found to follow 1st order kinetics. The doxorubicin was also released using an alternating magnetic field, this also followed 1st order kinetics with a rate constant of 1.7x10-2 min-1. This is four orders of magnitude greater than the thermal release at the same temperature (298 K). The work shows the magnetically controlled, burst release from a drug-loaded niosome delivery system. The release was triggered on demand by the application of the alternating magnetic field, resulting in 86% doxorubicin release within 3 hours.

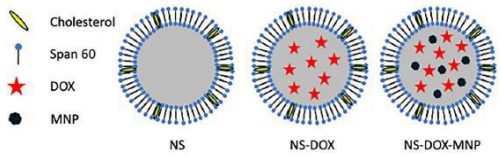

Fig. 1. An illustration of the niosome samples prepared. NS, DOX and MNP stand for niosome, doxorubicin and magnetic nanoparticles respectively.

Acknowledgements: This research was supported by the Royal Society of Chemistry (E22-5590558249), the University of Bradford and Airlangga University and the University of Leeds for electron microscopy and spectroscopy analysis and KFUPM for conference grant.

[1]Kazi, K. M.; Mandal, A. S.; Biswas, N.; Guha, A.; Chatterjee, S.; Behera, M.; Kuotsu, K. *J. Adv. Pharm. Technol. Res*., **2010**, *1*, 374.
[2]Izhar, M. P.; Hafeez, A.; Kushwaha, P.; Simrah. *J. Cluster Sci*., **2023**, *34*, 2257.
[3]Herrera, A. P.; Barrera, C.; Rinaldi, C. *J. Mater. Chem*., **2008**, *18*, 3650.
[4]Linh, P. H.; Phuc, N. X.; Hong, L. V.; Uyen, L. L.; Chien, N. V.; Nam, P. H.; Quy, N. T.; Nhung, H. T. M.; Phong, P. T.; Lee, I. J. *J. Magn. Magn. Mater*., **2018**, *460*, 128.
[5]Miatmoko, A.; Safitri, S. A.; Aquila, F.; Cahyani,D. M.; Hariawan, B. S.; Hendrianto, E.; Hendradi, E.; Sari, R. *Res. Pharm. Sc*i., **2021**, *16*, 660.

IM - D4 - P09
Exploring composite hydrogel systems using solid state NMR

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Hydrogels are structurally complex, heterogeneous polymer networks whose functional properties depend strongly on molecular-level interactions that remain challenging to characterise. In this work, solid-state nuclear magnetic resonance (ss NMR) spectroscopy is employed to investigate the structure and intermolecular interactions within a range of composite hydrogel systems based on poly(vinyl alcohol) (PVA).
Five hydrogel formulations were examined, including PVA–gelatin–chitosan composites, glutaraldehyde-crosslinked PVA with sodium alginate, PVA–TEOS hybrid networks with oxidized alginate, β-cyclodextrin-incorporated systems (Figure 1), and silica-supported flavylium dye-functionalised materials. ^{13}C CP/MAS NMR provided detailed insight into polymer backbone structure, crosslinking behaviour, and chemical environments, while ^{1}H ss NMR revealed changes in molecular mobility and hydrogen-bonding interactions.
Results indicate that, in the PVA–gelatin–chitosan system, interactions are predominantly non-covalent, with limited esterification under aqueous conditions. In contrast, glutaraldehyde and TEOS-based systems exhibit clear evidence of covalent crosslinking through acetal and siloxane linkages, respectively. Incorporation of oxidized alginate introduces additional hemiacetal/acetal structures, leading to increased network heterogeneity and reduced chain mobility. The inclusion of β-cyclodextrin and functional additives further modifies the hydrogen-bonding network and structural organisation, while immobilisation of flavylium dyes on silica demonstrates altered molecular environments and restricted mobility.
Overall, this study highlights the capability of ss NMR to resolve complex structural features in hydrogel systems, providing critical insight into the relationship between composition, intermolecular interactions, and material properties.

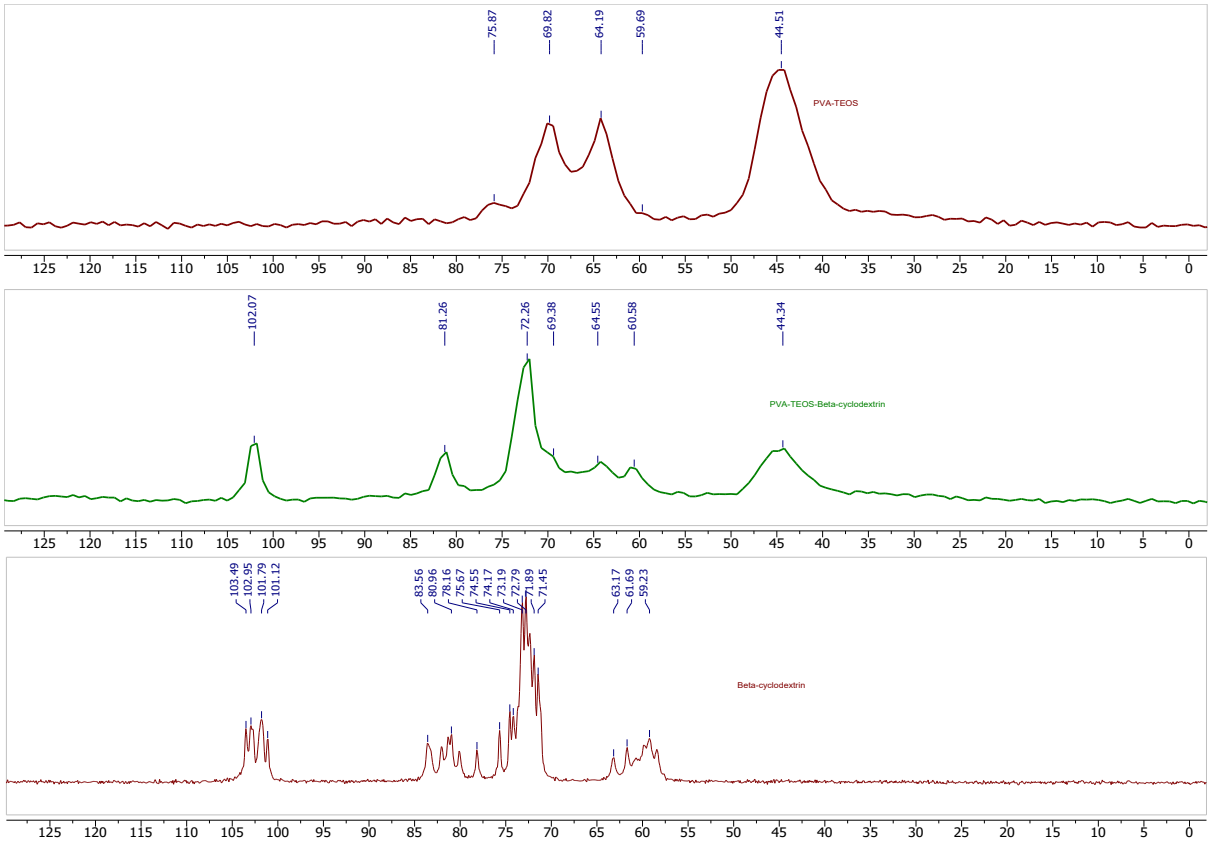

Fig.2. Stacked ss CP/MAS ^{13}C NMR spectra of PVA-TEOS film, PVA-TEOS film incorporated with cyclodextrin and of β-cyclodextrin

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[1]Ho, T.; Chang, C.; Chan, H.; Chung, T.; Shu, C.; Chuang, K.; Duh, T.; Yang, M.; Tyan, Y. Hydrogels: properties and applications in biomedicine. *Molecules* **2022,** *27* (9), 2902.
[2]Park, J.; Oh, Y.; Jeong, S.; Song, H.-W.; Choi, E.; Kim, H. Biobased Stimuli-Responsive Hydrogels That Comprise Supramolecular Interpenetrating Networks and Exhibit Programmed Behaviors. *Chem. Mater.* **2021**, *33*, 8124
[3]Wang, H.; Qu, G.; Liu, X.; He, M.; Yin, C.; Xu, R. Hydrogel materials in agriculture: A review. *J. Env. Chem. Eng.* **2025,** *13* (3), 116385.
[4]El-Sherbiny, I.; Yacoub, M. H. Hydrogel scaffolds for tissue engineering: progress and challenges. *Glob Cardiol Sci Pract.* **2013,** *3,* 316-342.
[5]Niemczyk-Soczynska, B.; Sajkiewicz, P. L. Hydrogel-based systems as smart food packaging: A Review *Polymers,* **2025,** *17* (8), 1005.
[6]Nonappa, Kolehmainen, E. Solid state NMR studies of gels derived from low molecular mass gelators. *Soft Matter* **2016,** *12* (28), 6015-6026.
[7]Moro, A:; Diniz, A. M.; Petrov, V.; Pina, F. Chemistry of 7,8-dihydroxy-2-(4-dimethylaminostyryl)-1-benzopyrylium - A photochromic system switching from yellow to green. *J. Photochem. Photobiol A* **2013,** *263,* 17-23.

IM - D4 - P10

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.

We acknowledge financial support from FAPESP Grants 2024/10984-2 and 2024/02935-1, Brazil.

IM - D4 - P11

Multifunctional novel materials for CO_2 capture and nutrient delivery: Advanced soil amendments to enhance soil health and crops growth

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This study presents the synthesis and evaluation of multifunctional materials (MFs) designed for simultaneous CO_2 capture and soil fertility enhancement, addressing challenges of desertification, carbon emissions, and poor soil productivity in arid regions. Composite formulations were prepared using sand, montmorillonite clay, humic acid, and charcoal, individually and in combination, with polyethyleneimine (PEI) surface modification to introduce amine-rich functional groups for improved chemisorption and nutrient interaction. Characterization through FTIR, XRD, SEM, and BET confirmed successful functionalization, enhanced surface area, and stable structural morphology. The materials displayed varying CO_2 adsorption capacities (0.025–4.5 mmol/g), with MF-12 achieving the highest performance due to synergistic interactions among PEI, clay, humic acid, and carbon phases. Water retention increased from 5% in pure sand to 38% in the best-performing composite. Electrical conductivity (0.406–0.537 mS/cm) remained within the optimal range for nutrient availability. In coriander growth trials, MF-12 demonstrated superior plant height, biomass, and petal development, confirming improved water retention and nutrient cycling. The study establishes that PEI-modified organic–inorganic composites are highly effective as multifunctional soil amendments capable of capturing atmospheric CO_2 while enhancing soil moisture, conductivity, and plant productivity, offering a sustainable solution for climate-resilient agriculture.

IM - D4 - P22

Systematic functionalization of silk sericin via acetylation: A design of experiments approach toward sustainable biomaterials

Rony Aad[1], Luca Leuzzi[2], Diletta Ami[2], Greta Bianchi[2], Marco Mangiagalli[2], Antonino Natalello[2], Laura Cipolla[2], Simone Vesentini[1]

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Silk sericin, the glue-like protein that binds fibroin fibers within silk, is generated in large quantities as an industrial byproduct and discarded despite its rich chemical functionality. Its intrinsic properties, including biocompatibility, biodegradability, antioxidant activity, and antibacterial behavior, make it a promising candidate for bio-based materials; however, its effective valorization remains limited by the lack of a quantitative understanding of the relationship between chemical modification and structural evolution. Here, a quantitative framework is established to investigate and control sericin functionalization using acetylation as a model reaction, which was selected for its ability to tune the degree of functionalization and secondary structure organization while introducing a biodegradable ester functionality. A Design of Experiments (DoE) approach was employed to systematically assess the effects of acetyl chloride equivalents, initial sericin concentration, and lithium chloride content, including their interaction effects. Fourier-transform infrared (FTIR) spectroscopy was advanced as a quantitative, model-integrated analytical approach. Band deconvolution across the Amide I region (1780–1580 cm^{-1}) enabled the extraction of two complementary descriptors, defined as the functionalization index (FI) and β-sheet index (BI), derived from band areas and intensities. The resulting models exhibited strong predictive capability and statistical significance ($p < 0.01$), with good agreement between experimental and predicted responses. Notably, the system displayed pronounced non-linear behavior governed by significant quadratic and interaction effects, revealing a multidimensional response surface. These findings demonstrate a direct coupling between chemical reactivity and protein structural organization, enabling predictive control over sericin modification. Overall, this work introduces a reproducible and quantitative methodology for linking reaction parameters to both chemical and structural outcomes, supporting the development of sericin as a sustainable, high-value biomaterial platform.

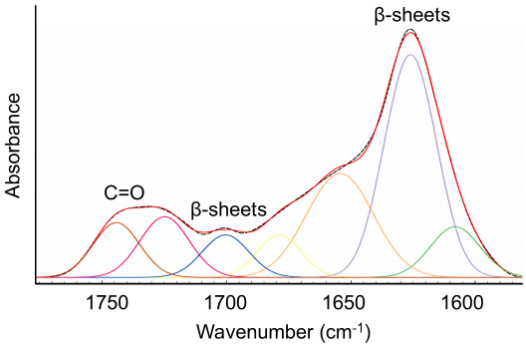

Fig.1. FTIR band deconvolution illustrating the extraction of functionalization and β-sheet structural descriptors.

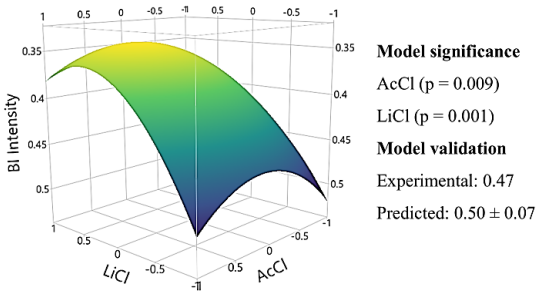

Fig. 2. Response surface of BI (intensity) highlighting the effects of AcCl and LiCl, with model significance and validation.

The 10th EuChemS Chemistry Congress

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Molecular Design & Reactivity (MDR)

MDR - D4 - P01
Molecular design of acrylic polymers for controlling the damping behavior of epoxy composites

Yong Rok Kwon[1], Jung Soo Kim[1], Sihun Jang[1], Dong Hyun Kim[1], Ju-Hee So[1,*]
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Epoxy-based composites are widely used in semiconductor packaging processes due to their excellent mechanical strength and thermal stability. However, they are susceptible to interfacial delamination and cracking under thermal cycling conditions, where repeated stresses are generated. In particular, for semiconductor post-processing film materials, including die-attach films, the ability to relax stresses arising from the coefficient of thermal expansion mismatch between the chip and the substrate is a critical factor governing long-term reliability.
From this perspective, this study aims to systematically investigate the effects of the glass transition temperature (Tg) and molecular weight (Mw) of acrylic polymers on the damping behavior of epoxy composites. Acrylic polymers with controlled Tg and Mw were synthesized and incorporated into epoxy resins, and the resulting composites were evaluated using dynamic mechanical analysis. The storage modulus, loss modulus, and tan δ responses were analyzed to characterize the viscoelastic behavior of the systems. In particular, the position, width, and area of the tan δ peak were analyzed in detail to evaluate the damping characteristics that are closely related to stress relaxation. Through this approach, this work seeks to identify key acrylic polymer design parameters for achieving the thermal cycling reliability required in semiconductor post-processing films and to provide fundamental insights into structure–property relationships of epoxy-based film materials from a damping perspective.

MDR - D4 - P02
The design & synthesis of fluorescent self-assembled monolayers for optical applications

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Controlling the orientation of π-conjugated molecules is an important area of research, as molecular orientation plays a critical role in determining the efficiency of optoelectronic devices.[1] However, many high-performance devices are currently fabricated using vacuum evaporation techniques, which are energy intensive and suffer from extremely low material utilisation.[2] Developing alternative, solution-processed routes that enable precise control over molecular orientation therefore represents an attractive and more sustainable strategy.
In this work, we introduce a novel approach towards controlling molecular orientation based on greener, solution-processed methods. The control of tilt angle within self-assembled monolayers (SAMs) is exploited to influence the orientation of π-conjugated molecules at transparent conducting oxide interfaces. A series of carbazole donor–acceptor emitters were designed and synthesised, with particular emphasis placed on achieving the high levels of purity required for reliable self-assembly.
Monolayers were deposited onto indium tin oxide (ITO) substrates, and their formation and organisation were investigated using a combination of X-ray photoelectron spectroscopy (XPS) and other surface characterisation techniques. These techniques reveal high binding efficiencies, and the effects of deposition parameters and post-deposition treatment on film quality and surface coverage was also examined.
Finally, the effect of surface binding and molecular orientation on photophysical behaviour was investigated. Solution-phase studies show bright blue charge-transfer emission with solvatochromic behaviour, while solid-state measurements are ongoing but indicate bright emission. Future work will demonstrate how controlled self-assembly at oxide surfaces can be used to tune optical behaviour, highlighting the potential of SAM-based strategies for the development of efficient, sustainable optoelectronic devices.

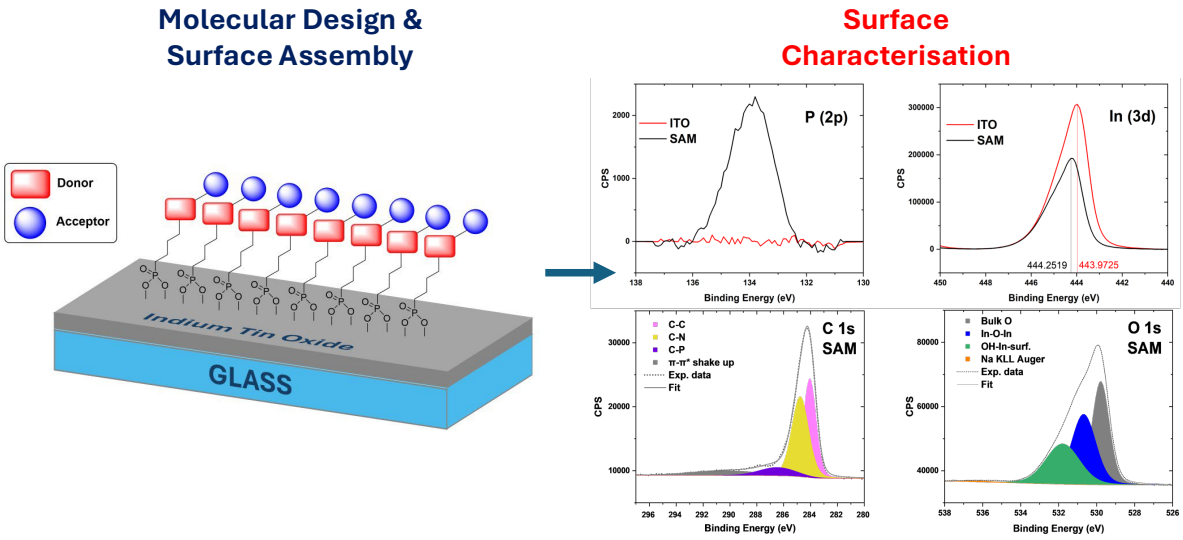

Fig. 1. Left: Schematic representation of donor–acceptor self-assembled monolayers (SAMs) on ITO. Right: XPS spectra confirming SAM binding to the ITO surface.

[1]Schmidt, T. D.; Lampe, T.; R, D. S. M.; Djurovich, P. I.; Thompson, M. E.; Brütting, W., *Phys. Rev. Appl.* **2017**, *8* (3), 037001
[2] Lee, T.; Noh, T.; Shin, H.; Kwon, O.; Park, J.; Choi, B.; Kim, M.; Shin, D. W.; Kim, Y., *Adv. Funct. Mat.,* **2009**, *19* (10), 1625–1630.

MDR - D4 - P03

Synthesis and evaluation of boronate precursors for stable astatine radiopharmaceuticals

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Fibroblast activation protein (FAP) targeting of radionuclides is investigated as a therapeutic strategy in many domains of oncology. UAMC-1110, a potent and highly selective FAP-inhibitor discovered in our group, is widely used as a FAP-targeting vector in clinically developed oncology theranostics.[1,2] One of the underrepresented radionuclides in this effort is ^{211}At. This alpha-emitting radionuclide is of great interest to nuclear medicine due to its ability to induce irreversible cell death in tumors. Introducing it in a metabolically stable form into a radiopharmaceutical, however, is an enduring challenge.[3] A major limitation for *in vivo* applications is de-astatination, a phenomenon where a carbon–astatine bond is cleaved, leading to suboptimal tumor irradiation and off-target accumulation of free astatine in healthy tissue.

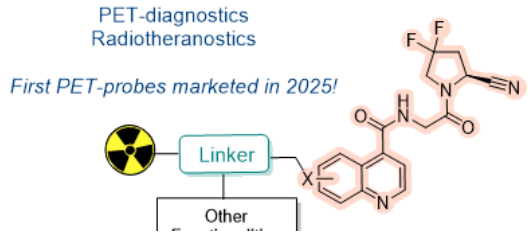

Fig.2. FAP-targeting radiotheranostics

To effectively tackle this problem, we propose innovative astatine-bearing prosthetic groups and that allow chemical stabilization of the C-At bond by modifying the electronic and steric properties.

A first series of boronic precursors has been synthesized for radiolabeling. Boron-based precursors were selected since our group was successful in optimizing astatination yields with this type of compounds. An additional advantage is that boronate cross-coupling chemistry is extremely well documented because of the importance of Suzuki-Miyaura chemistry. The synthesis of these boronic precursors, nonetheless, came with several challenges, which were solved through optimization and application of literature-reported techniques.

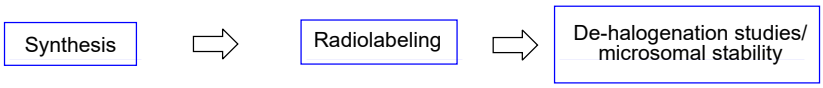

Fig. 3. *De-astatination stability screening cascade*

The resulting fragments were radiolabeled with ^{211}At and screened *in vitro* for their resistance to de-astatination.[4] This experimental effort is backed with Density Functional Theory (DFT)-based bond dissociation energy (BDE) calculations, to find the optimal substitution for C-At bond stability. Ultimately, the goal is to assess optimized stable ^{211}At-FAPi radiotheranostic compounds in preclinical mouse models.

[1]Jansen, K., Heirbaut, L., Verkerk, R., Cheng, J. D., Joossens, J., Cos, P., ... & Van der Veken, P. **2014**, Journal of medicinal chemistry, 57(7), 3053-3074.
[2]Van Rymenant, Y., Tanc, M., Van Elzen, R., Bracke, A., De Wever, O., Augustyns, K., ... & Van Der Veken, P. **2021**. Frontiers in Chemistry, 9, 640566.
[3]Mador, S. D., Yssartier, T., Le Questel, J. Y., Montavon, G., Guérard, F., & Galland, N. **2025**, *ACS Physical Chemistry Au*.
[4]Fouinneteau, R., Maingueneau, C., Galland, N., Perrio, C., & Guérard, F. **2025**. *Scientific Reports*, *15*(1), 16877.

MDR - D4 - P04

Ring-opening polymerization of δ-tetradecalactone for oil-soluble poly(ester) lubricant additives with tunable molecular weight

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Cyclic lactones bearing long alkyl substituents represent an effective platform for oil-soluble polymeric lubricant additives due to the coexistence of polar ester functionalities and hydrocarbon-compatible side chains. In this work, δ-tetradecalactone (δ-TDL), a C14-substituted δ-lactone, was investigated as a monomer for the preparation of poly(ester)-based lubricant additives via ring-opening polymerization (ROP). Polymer architectures with controlled molecular weight were achieved by regulating the monomer-to-initiator ratio, enabling the preparation of multiple polymer grades spanning low to high molecular weight regimes. The synthesized polymers were characterized by nuclear magnetic resonance spectroscopy and gel permeation chromatography, confirming monomer conversion, chain structure, and effective molecular weight control with narrow dispersity. Lubricant formulations containing the polymers were prepared by blending into commercial base oils at low treat rates. The viscosity–temperature behavior was evaluated through kinematic viscosity measurements, and viscosity index (VI) enhancement was observed as a function of polymer molecular weight. Low-temperature flow behavior was evaluated by pour point measurements, where a noticeable depression of the pour point was observed in polymer-containing lubricant formulations relative to the neat base oil.
The long alkyl side chain of δ-TDL contributed to excellent oil solubility and compatibility, while the ester backbone provided polar interactions with metallic surfaces, supporting both thickening efficiency and boundary lubrication performance. These results demonstrate that lactone-derived polymeric additives constitute a versatile and tunable design platform for lubricant applications, where molecular weight and polymer architecture play a critical role in determining macroscopic performance.

Acknowledgements: This work was supported by the Technology Innovation Program (Parts and Materials Technology Development) under Grant RS-2024-00433164, funded by the Ministry of Trade, Industry and Energy (MOTIE, Republic of Korea).

MDR - D4 - P05

Epoxy-terminated polyurethanes as effective toughening agents for epoxy molding compounds

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A toughening agent is an additive incorporated into epoxy resins to absorb and dissipate applied stress, thereby improving the material's toughness. Although epoxy resins exhibit excellent mechanical and thermal properties, their inherent brittleness limits practical applications. Therefore, epoxy-terminated polyurethanes (EPUs) were employed as toughening agents to overcome this drawback.

EPUs were synthesized via bulk polymerization of isophorone diisocyanate and polyols, followed by the introduction of glycidol for epoxy end-functionalization of the polymer chains. Three different polyols, polyethylene glycol, polypropylene glycol (PPG), and polytetrahydrofuran, were employed as variables to investigate the properties of the EPUs. The synthesized EPUs were characterized by Fourier transform infrared spectroscopy, which confirmed urethane linkage and the introduction of epoxy functional groups. The mechanical properties and viscoelastic behavior were evaluated using tensile testing and dynamic mechanical analysis. Thermal properties were analyzed by differential scanning calorimetry and thermogravimetric analysis. Furthermore, scanning electron microscopy was utilized to examine fracture morphologies, providing insight into the toughening mechanism. The PPG-based EPU exhibited the highest enhancement in toughness of epoxy resins, as revealed by a comparative evaluation of EPUs prepared with different polyols. Based on these toughening effects, EPUs are expected to serve as effective toughening agents for epoxy systems requiring improved toughness, such as epoxy molding compounds.

MDR - D4 - P06

Toughening effect of core-shell impact modifiers on epoxy resin maintaining thermal stability

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Impact modifiers are widely used to enhance the toughness of thermosetting polymer resins, including epoxy (EP), by improving energy dissipation and crack resistance. Among them, liquid rubbers enhance the toughness of EP. However, their incomplete phase separation reduces thermal stability of EP, such as glass transition temperature (T_g). Therefore, core-shell impact modifiers (CSIMs) have been studied to improve the toughness of EP while maintaining thermal stability. Two types of CSIMs were synthesized via semi-batch emulsion polymerization: non-reactive CSIM and reactive CSIM. Both CSIMs use butyl acrylate as the core monomer. The core was synthesized by seed emulsion polymerization, then the shell was synthesized on the surface of the core via semi-batch emulsion polymerization. For the shell, non-reactive CSIM used methyl methacrylate (MMA), while reactive CSIM used a copolymer of MMA and glycidyl methacrylate (GMA). The reason why GMA is applied in reactive CSIM is that its epoxy functional groups provide high compatibility with EP resin and react with the curing agent. The core-shell structure of CSIMs was characterized by using transmisiion electron microscopy. The thermal properties of CSIM applied EP were evaluated using differential scanning calorimetry and thermogravimetric analysis, while their mechanical properties were examined through impact and flexural test. The impact and flexural strength of EP with reactive CSIM have improved without a significant decrease in T_g compared to neat EP and EP with non-reactive CSIM, which is attributed to the epoxy groups of GMA present in the shell participating in the curing reaction of EP resin, enhancing the cross-linking density. The dispersibility of the CSIM was verified by observing the fracture surface of the composites under scanning electron microscopy.

MDR - D4 - P07

Theoretical design principles for spin-selective relaxation in photoexcited metal complexes

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Electron spin polarization in molecular systems is a phenomena where the non-Boltzmann population distribution among spin sublevels of electronic states with spin multiplicity greater than two. In recent years, it has attracted considerable attention from the perspective of quantum control technologies, such as optically detected magnetic resonance (ODMR) and dynamic nuclear polarization (DNP). Although various mechanisms for generating electron spin polarization have been proposed—some still at the hypothesis stage—one relatively reliable mechanism is spin-selective intersystem crossing (SS-ISC). In the SS-ISC mechanism, for example, photoexcitation of pentacene generates an excited singlet (S1) state, and during intersystem crossing to a nearby excited triplet (T2) state, differences in transition rates to the three spin sublevels T2(X), T2(Y), and T2(Z) produce spin polarization in T1. These differences in transition rates are considered to originate from the anisotropy of spin–orbit coupling (SOC), which mediates the spin-forbidden intersystem crossing process.

In this study, we theoretically predict photoinduced spin polarization in metal complexes with triplet ground states. Three complexes—Cr(o-tolyl)$_4$ (1-Cr), $(C_6F_5)_3$trenVCNtBu (2-V), and $^{Me}Tp_2Ni$ (3-Ni)—were investigated. The energies of low-lying excited states, spin–orbit coupling matrix elements between relevant states, and zero-field splitting (ZFS) parameters necessary for predicting spin polarization were calculated using multireference electronic structure theory, namely the complete active space self-consistent field (CASSCF) method and second-order perturbation theory on top of the CASSCF (CASPT2). In addition, the spin selectivity of intersystem crossing was analyzed from a group-theoretical perspective including molecular vibrational modes, and the results were compared with the calculated SOC matrix elements.

The calculated ZFS parameters for all complexes were sufficiently small to allow microwave manipulation. For 1-Cr and 2-V, excited singlet states were found to lie below the lowest excited triplet state, and the anisotropy of the SOC matrix elements suggests that spin-selective intersystem crossing can occur. Furthermore, we theoretically investigated the spin selectivity of relaxation processes from singlet states to the triplet ground state, incorporating vibronic coupling effects. Finally, we propose molecular design strategies to enhance spin selectivity beyond that achievable through vibronic interactions alone.

[1] K. Sakamoto, et.al., *Proc. Natl. Acad. Sci. U.S.A.* **2023**, 120 (44), No. e2307926120.
[2] M. S. Fataftah, et.al. *Chem. Comm.* 2018, **54**, 13773.
[3] S. L. Bayliss, et.al. *Science* 2020, **370**, 1309.

MDR - D4 - P08
Improving the toughness of electronic adhesives through epoxy-acrylic hybridization

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Epoxy resin is a representative thermosetting polymer that is widely used for electronic and semiconductor adhesives, high-reliability structural adhesives, surface coatings, paints, protective layers, owing to its excellent adhesion, high mechanical strength, outstanding chemical and corrosion resistance, and good electrical properties. However, the high crosslink density of epoxy resins can embrittle the material, thereby reducing resistance to crack initiation and propagation. In particular, in structural and electronic adhesive applications where interfacial stress concentration occurs, such brittleness can lead to fracture or delamination, which is a major factor limiting the application of epoxy resins. To overcome these limitations, acrylic rubber with a saturated backbone and various pendant groups has been widely used as a toughness modifier for epoxy resins. In this study, acrylic rubbers with varying epoxy-group content were synthesized by controlling the glycidyl methacrylate (GMA) content, and adhesive films were prepared by blending the acrylic rubbers with an epoxy resin and a curing agent. The acrylic rubbers were synthesized using butyl acrylate (BA), 2-hydroxyethyl acrylate (HEA), methyl methacrylate (MMA), and GMA as monomers. BA and MMA were used to tailor the flexibility and stiffness of the acrylic rubber, and HEA was introduced to enhance adhesion to substrates through hydroxyl groups. GMA is an epoxy-functional monomer that enables the formation of chemical bonds with the epoxy matrix and can enhance compatibility. The effects of epoxy-group content on the toughness and thermomechanical properties of the epoxy/acrylic-rubber adhesive films were systematically evaluated. The toughness and adhesion strength of the adhesive films were evaluated using tensile and T-peel tests. Furthermore, the thermal and viscoelastic behaviors of the adhesive films were analyzed using differential scanning calorimetry and dynamic mechanical analysis.

MDR - D4 - P09

General and selective ruthenium-catalyzed hydrogenation of primary amides to primary amines under mild conditions

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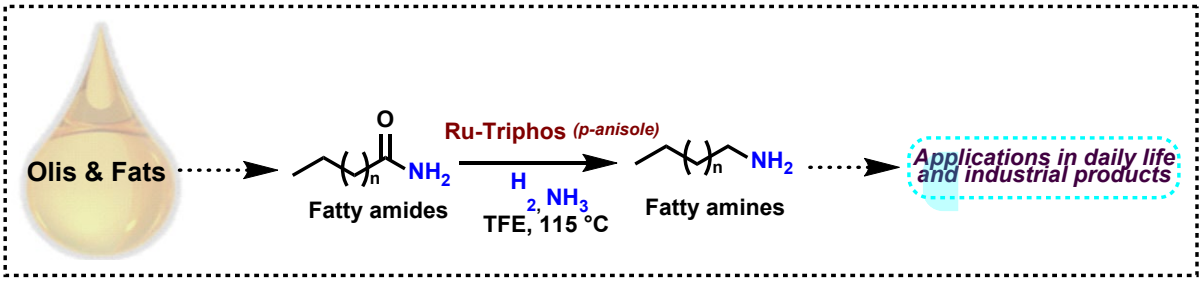
Catalytic hydrogenations are an essential class of synthetic processes, which are widely used in both research laboratories and industries to produce fine and bulk chemicals as well as pharmaceuticals, and agrochemicals.[1,2] Hydrogenation of amides continues to be one of the most difficult reductive transformations in organic synthesis.[3,4] Despite significant efforts in past decades, there is no general protocol reported allowing the synthesis of various primary amines from the corresponding primary amides using molecular hydrogen. To perform this challenging reaction, here we report a specific homogeneous ruthenium catalyst based on the methoxy-substituted triphos ligand (Triphos(p-anisole)). In the presence of this Ru-catalyst system, industrially relevant, functionalized, and structurally diverse aromatic, heterocyclic and aliphatic primary amides including fatty amides were selectively hydrogenated to produce the corresponding primary amines under comparably mild conditions (typically 115 °C and 10 bar H_2). The resulting amines are valuable compounds with diverse applications in chemistry, medicine and biology as well as in materials and energy technologies.



Acknowledgements: We thank the German Research Foundation (DFG project numbers 670389-NFDI2/1 and 447724917), and the State of Mecklenburg-Vorpommern for financial and general support. We gratefully acknowledge the financial support from the European Union under the REFRESH-Research Excellence or Region Sustainability and High-tech Industries project number CZ.10.03.01/00/22_003/0000048 via the Operational Programme Just Transition. Vishakha Goyal acknowledges the financial support of the European Union under the “MSCA Fellowships CZ at VSB-TUO 2.0” project, reg. nr. CZ.02.01.01/00/22_010/0008714 within the Johannes Amos Comenius Operational Programme. We are thankful to the analytical team of the Leibniz-Institut für Katalyse e.V. for their excellent service.

[1]Nishimura, S. Handbook of heterogeneous catalytic hydrogenation for organic synthesis, **2001**, *Wiley-VCH*, 290-291.
[2]Vries de, J. G.; Elsevier, C. J. The handbook of homogeneous hydrogenation, **2007**, *WILEY-VCH Verlag GmbH & Co. KGaA* .
[3]Cabrero-Antonino, J. R.; Adam, R.; Papa, V.; Beller, M. *Nat. Commun.* **2020**, 11, 3893.
[4]Pattabiraman, V. R.; Bode, J. W. *Nature*, **2011**, 480, 471-479.

MDR - D4 - P10

Structure activity relationship directed development of an internal standard for an electrochemical fentanyl detector

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Between 2016 and 2023, Canada experienced 44,592 opioid-related deaths, making opioids the leading cause of accidental death among Canadians under 65.[1,2] Despite their addictive potential, opioids remain essential for pain management, palliative care, and end-of-life care.[3,4] Since 2013, the prevalence of fentanyl and other potent synthetic opioids has accelerated overdose rates.[5] Fentanyl, with a potency 100–200 times greater than morphine,[6] accounted for 83% of opioid overdose deaths in Canada in 2023.[1]

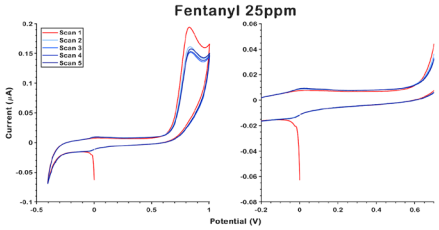

Figure 1: Fentanyl CV

To address the need for rapid fentanyl detection, this work develops a point-of-use electrochemical detector for fentanyl quantification in biological fluids and illicit drug samples. Detecting trace fentanyl in illicit substances can enhance harm-reduction efforts by improving drug testing reliability. Key features include high-throughput screening (<5 min analysis time with concurrent processing), ease of use, compact design, cost efficiency, and a detection threshold exceeding current field-deployable methods.

A key challenge is the lack of a suitable internal standard with electrochemical behavior comparable to fentanyl. To address this, novel fentanyl analogues were synthesized with targeted structural modifications to tune redox potentials while reducing opioid potency. Over 50 analogues were prepared, identifying three candidates with redox signals offset by approximately ±0.3 V from fentanyl's signal at 0.08 V. Ongoing work includes evaluation in mixed drug samples, and studies in biologically relevant matrices.

[1]Lofton, A. *Encyclopedia of Toxicology*, 2nd ed.; Elsevier: New York, 2005; pp 322–324.
[2]Statistics Canada. *The Daily—Deaths, 2021.* https://www150.statcan.gc.ca/n1/daily-quotidien/230828/dq230828b-eng.htm.
[3]Marchand, L. R. *Integrative Medicine*; Elsevier, 2018; pp 806–816.e4.
[4]Hammack, J. E.; Loprinzi, C. L. *Mayo Clin. Proc.* **1994**, *69*, 384–390.
[5]Rudd, R. A.; Aleshire, N.; Zibbell, J. E.; Gladden, M. R. *Morb. Mortal. Wkly. Rep.* **2016**, *64*, 1378–1382.
[6]Stanley, T. H. *J. Pain* **2014**, *15*, 1215–1226.

MDR - D4 - P11

Monomer structure and feed protocol effects on microstructure and processing of resorcinol based polyarylates

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Resorcinol based polyarylates intrinsically absorb UV radiation through aromatic arylate chromophores, enabling built in UV screening. Under UV exposure, arylate linkages can undergo a photo-Fries rearrangement to form o-hydroxybenzophenone derivatives that may contribute to sustained UV absorption during ageing. Beyond overall composition, the sequence distribution established during solution polycondensation can influence segmental heterogeneity, glass transition temperature characteristics, and solution processing behaviour. Here, we evaluate how aliphatic diol architecture and monomer addition order jointly control microstructure and properties in resorcinol based polyarylates.

Polyarylates were synthesized from aromatic diacid chlorides and resorcinol together with one of two aliphatic diols providing contrasting conformational rigidity: a cyclic (stiff) diol and a linear (flexible) diol. For each aliphatic diol, three feed protocols were applied at identical target stoichiometry: (i) one pot polymerization using a premixed diol blend, (ii) sequential addition with resorcinol introduced first, and (iii) sequential addition with the aliphatic diol introduced first. We hypothesize that differences in relative diol reactivity during early oligomer formation generate protocol dependent sequence distributions, while monomer architecture sets the baseline chain stiffness.

The resulting polymers were comprehensively characterized by NMR, FTIR, UV-Vis, GPC, DSC to correlate molecular architecture with thermal transitions. Standardized solubility and precipitation tests were used to compare aggregation and isolation behaviour. The study demonstrates that varying the feed protocol allows for tuning of segmental blocks, which directly modulates solution processability and solvent polymer interactions without compromising the intrinsic UV absorbing character. By controlling the sequence distribution, we report a route to engineer polyarylates with tailored solubility profiles, offering a advantage for specialized coating applications and thin film processing.

MDR - D4 - P12

A mechanochemical Kolbe-Schmitt reaction: Catechol carboxylation provides building blocks for renewable plasticizers

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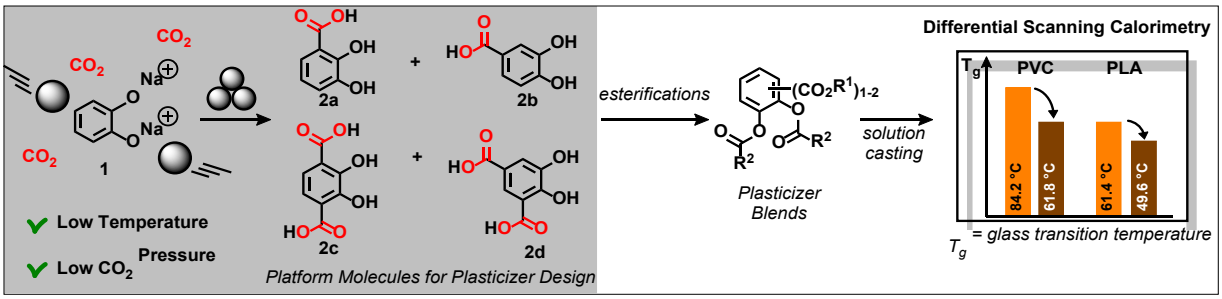
Catechol, produced annually at 40 ktons, is a key commodity chemical prepared from phenol derived from crude oil.[1] Recently, it has been derived from non-edible biomass in biorefineries, offering a renewable alternative to fossil carbon for chemical production.[2-6] An interesting transformation is its carboxylation with the greenhouse gas CO_2 as a C1-reactant, thereby allowing to generate dihydroxybenzoic acids with 100% renewable carbon featuring handles for further derivatization. However, the classical Kolbe-Schmitt reaction of disodium catecholate (**1**) with CO_2 requires harsh reaction conditions involving high temperature (up to 225 °C) and CO_2 pressures (up to 76 bar).[7-8] In this work, disodium catecholate (**1**) was carboxylated by mechanochemical Kolbe-Schmitt reaction with CO_2, providing a mixture of mono- and dicarboxylated catechol derivatives (**2a**-**2d**) at room temperature under low CO_2 pressure (4 bar).[9]
From the individual catechol-based mono- and dicarboxylic acid reaction products, a library of renewable plasticizers was synthesized through esterification of the carboxylic acid and the phenolic hydroxy groups. The resulting esters were evaluated as plastic additives in poly(vinylchloride) (PVC) and poly(lactic acid) (PLA), revealing plasticizing efficiencies competitive to commercial plasticizers.[9] The best performing substitution pattern was also effective when applied to the ball mill-derived mixture of mono- and dicarboxylated catechols, eliminating the need for resource-intensive (chromatographic) separation.



[1] Wu, X.; Smet, E., Brandi, F.; Raikwar, D.; Zhang, Z.; Maes, B. U. W.; Sels B. F. *Angew. Chem. Int. Ed.* **2024**, *63*, e202317257.
[2] Bomon, J.; Van Den Broeck, E.; Bal, M.; Liao, Y.; Sergeyev, S.; Van Speybroeck, V.; Sels, B. F.; Maes, B. U. W. *Angew. Chem. Int. Ed.* **2020**, *59*, 3063–3068.
[3] Bomon, J.; Bal, M.; Achar, T. K.; Sergeyev, S.; Wu, X.; Wambacq, B.; Lemière, F.; Sels, B. F.; Maes, B. U. W. *Green Chem.* **2021**, *23*, 1995–2009.
[4] Wu, X.; Liao, Y.; Bomon, J.; Tian, G.; Bai, S.-T.; Van Aelst, K.; Zhang, Q.; Vermandel, W.; Wambacq, B.; Maes, B. U. W.; Yu, J.; Sels, B. F. *ChemSusChem,* **2022**, *15*, e202102248.
[5] Bocus, M.; Van Den Broeck, E.; Wu, X.; Bal, M.; Bomon, J.; Vanduyfhuys, L.; Sels, B.F.; Maes, B. U. W.; Van Speybroeck, V. *Nat. Catal.* **2025**, *8*, 33–45.
[6] Wu, X.; Bal, M.; Zhang, Q.; Bai, S.-T.; Scodeller, I.; Vermandel, W.; Yu, J.; Maes, B. U. W.; Sels, B. F. *J. Am. Chem. Soc.* **2025**, *147*, 4915–4929.
[7] Chen, B. C.; Bednarz, M. S.; Sundeen, J. E.; Zhang, Z. J.; Caulfield, T. J.; Bisacchi, G. S. *Org. Prep. Proced. Int.* **1999**, *31*, 106–109.
[8] Mohammed, O.; Onwudili, J. A.; Yuan, Q.; Evans, R. *Chem. Eng. J.* **2025**, *515*, 163498.
[9] De Vos, D.; Pfennig, V. S.; Goddé, A.; Vroemans, R.; Krückel, T.; Marcinkowska, N.; Bartalucci, E.; Wiegand, T.; Bolm, C.; Maes, B. U. W. *Angew. Chem. Int. Ed.* **2026**, e19827.

MDR - D4 - P13

Two electrons in a Li-S C-cage: A novel lithium cubic electride - $[(tBu_2MeSiS)_6Li_8]^{2+}\bullet 2e^-$

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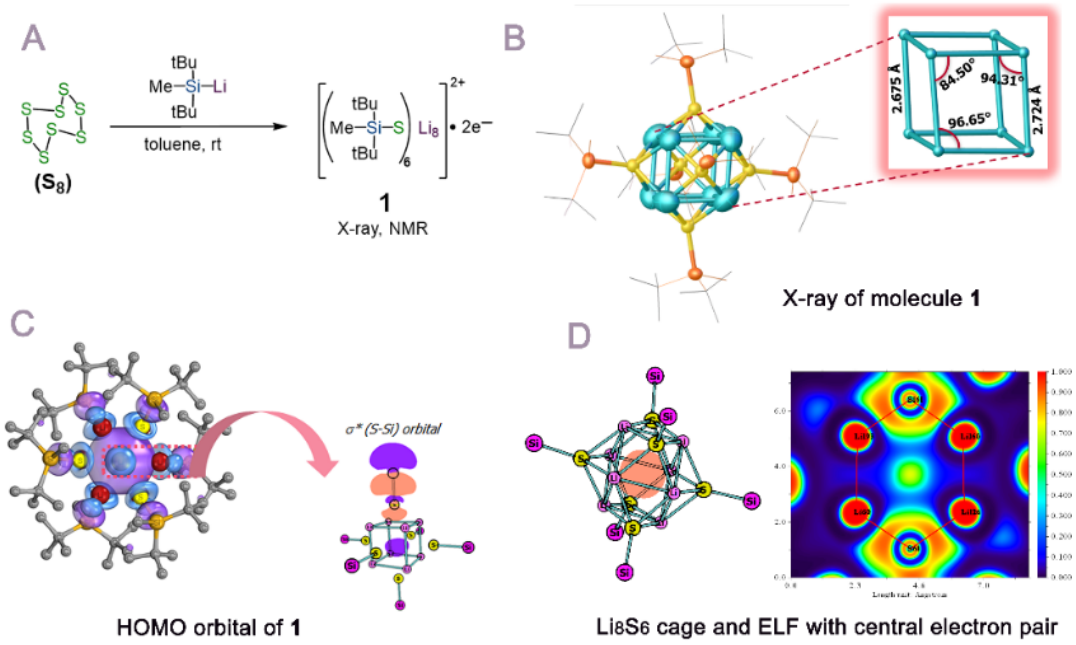
Electrides - materials in which electrons serve as anions, are of fundamental importance for catalysis, energy storage, and quantum materials owing to their exceptional electron-donor properties.[1-2] However, despite extensive progress in solid-state systems, the realization of thermally stable, single-molecule electrides with centrally stored electrons has remained a major synthetic challenge. In 2003, Matsuishi *et al.* reported the first thermally stable electride $[Ca_{24}Al_{24}O_{64}]^{4+}\bullet 4e^-$, formed by removing central O^{2-} ions from extended oxide cages, thereby enabling electron confinement within the nanoporous framework.[3] While such solid-state electride materials are well studied, singly isolated electrides with high thermal stability and truly central electron(s) remain mostly unknown.

Here we report an unprecedented lithium–sulfur–silyl cluster, $[(tBu_2MeSiS)_6Li_8]^{2+}\bullet 2e^-$, (**1**) - the **first thermally stable and structurally characterized molecular electrides featuring confined interstitial electrons** (Scheme 1, A-B). X-ray and ELF analyses confirm the confinement of an interstitial electron pair within the S_6Li_8 cluster (Scheme 1, D) and the cubic Li_8 cavity of 15.23 Å^3. NBO data reveal dominant contributions from Li(ry) and σ*(S–Si) orbitals (Scheme 1C). The electride-like HOMO is high-lying (–1.66 eV) and the HOMO–LUMO gap is small (1.17 eV), indicating strong central electron localization. To the best of our knowledge, **no electrides with high electron density inside a single-isolated molecule cage have been previously reported.** Our findings establish a molecular design paradigm where cavity volume, ligand architecture, and orbital diffuseness can be tuned to access structurally stable, solution-processable molecular electrides.



Scheme 1. (A) Synthesis of **1**; (B) X-ray structure of **1**, showing a Li_8 cubic arrangement; (C) HOMO orbital of **1**, showing σ* (S-Si) orbital contribution; (D) Electron Localized Function (ELF) graph of the Li_8S_6 cage showing the central electron pair density.

[1]H. Hosono, M. Kitano, *Chem. Rev*. **2021**, *121*, 3121−3185.
[2]D. L. Druffel, A. H. Woomer, K. L. Kuntz, J. T. Pawlik, S. C. Warren, *J. Mater. Chem. C* **2017**, *5*, 11196.
[3]S. Matsuishi, Y. Toda, M. Miyakawa, K. Hayashi, T. Kamiya, M. Hirano, I. Tanaka, H. Hosono, *Science* **2003**, *301*, 626−629.

MDR - D4 - P14
Expanding drug-relevant chemical space through Pt-Au bimetallic catalysis

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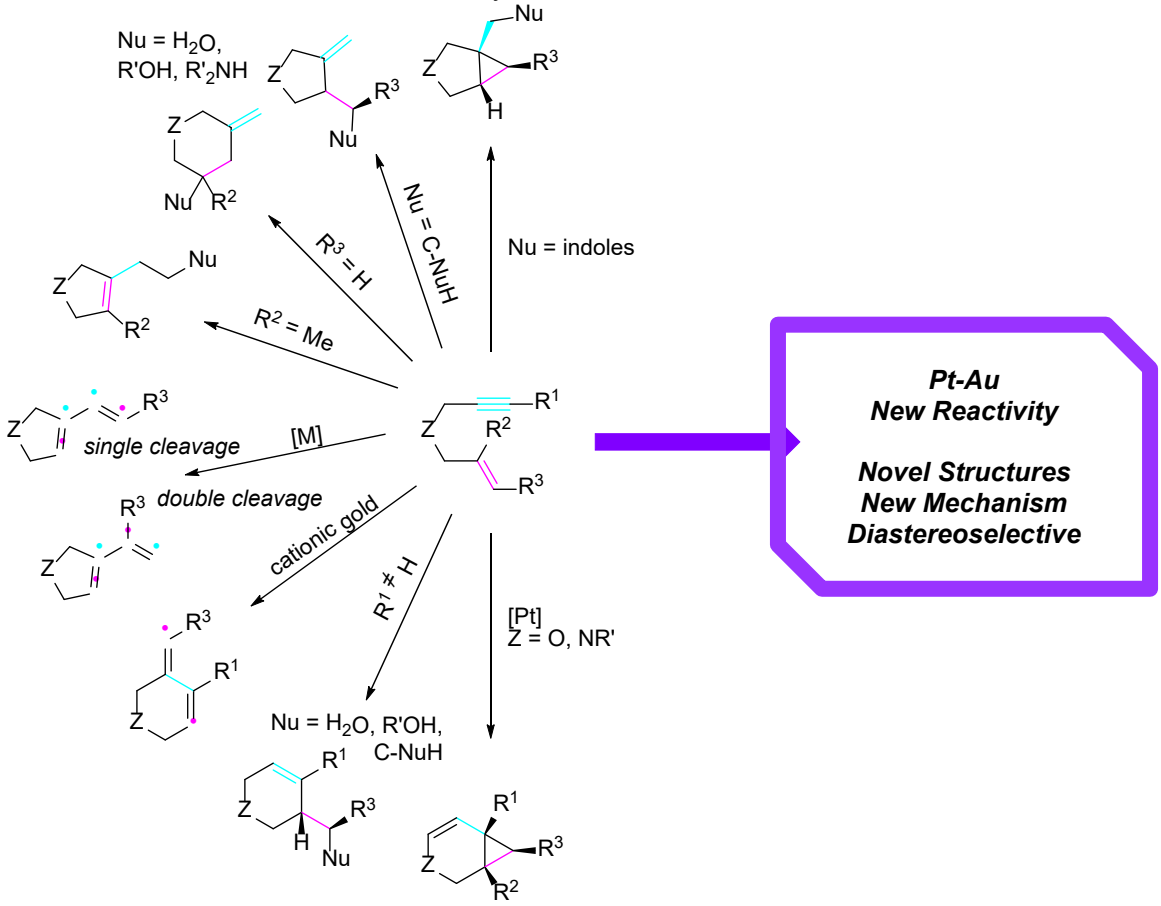
Bimetallic catalysis has evolved in recent years as a powerful strategy towards the synthesis of new structures, inaccessible through monometallic systems. Homogeneous Pt-Au bimetallic catalysis has scarcely been reported on, except for by Muñoz and co-workers,[1,2] to achieve novel, azole-containing compounds with promising antimicrobial activity.[3] The key to the enhanced and divergent reactivity established here is due to the highly electrophilic bimetallic carbene intermediate,[4] and, thus, applying this new methodology to known systems that proceed via a gold carbene intermediate should unlock new possibilities. 1,6-Enynes have been known to undergo several different reactions, including the nucleophilic addition of indoles.[5-7] Under Pt-Au bimetallic catalysis, new interactions with 1,6-enynes have been discovered to give divergent reactivity to access new structures diastereoselectively.



[1] J. M. Alonso and M. P. Muñoz, *Org. Lett.*, 2019, **21**, 7639-7644.
[2] J. M. Alonso and M. P. Muñoz, *Angew. Chem. Int. Ed.*, 2018, **57**, 4742-4746.
[3] M. P. Muñoz, *Unpublished results*.
[4] J. M. Alonso and M. Paz Muñoz, *ChemCatChem*, 2018, **10**, 2646-2654.
[5] C. H. M. Amijs, V. López-Carrillo, M. Raducan, P. Pérez-Galán, C. Ferrer and A. M. Echavarren, *J. Org. Chem.,* 2008, **73**, 7721-7730.
[6] C. Obradors and A. M. Echavarren, *Acc. Chem. Res.*, 2014, **47**, 902-912.
[7] E. Jiménez-Núñez and A. M. Echavarren, *Chem. Rev.*, 2008, **108**, 3326-3350.

MDR - D4 - P16

Heck coupling of 10,10'-dibromo-9,9'-bianthracene with para-substituted styrenes

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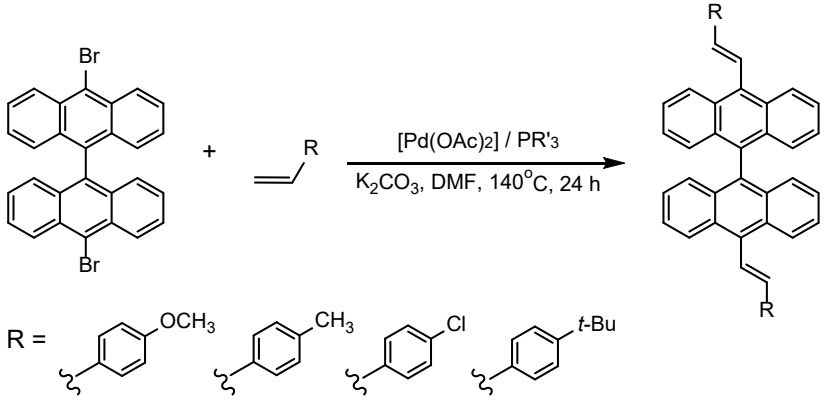
Anthracene and bianthracene derivatives play a key role in modern materials chemistry due to their unique photophysical properties, which make them suitable for applications in organic light-emitting diodes (OLEDs)[1] and organic field-effect transistors (OFETs)[2]. One of the most important methods enabling their functionalization is the Heck coupling reaction[3], which is widely used in both organic synthesis and materials chemistry, for example in the preparation of monomers for electronic layers[4].
The aim of this study was to develop a highly selective and efficient procedure for the synthesis of targeted polyunsaturated compounds. Our attention was focused on catalytic systems based on palladium complexes in the presence of Buchwald phosphine ligands and on the investigating the of coupling reactions of 10,10′-dibromo-9,9′-bianthracene with para-substituted styrenes (Scheme 1)[5].



Scheme 1. Synthesis of 10,10'-bis(E-styryl)-9,9'-bianthracenes.

The obtained products were isolated and characterized using ^{1}H and ^{13}C NMR spectroscopy as well as mass spectrometry. For selected compounds, crystal structures were additionally determined. The results clearly confirm that the Heck coupling reaction constitutes an effective and versatile tool for the synthesis of unsaturated 9,9′-bianthracene derivatives with promising luminescent properties, suitable for applications in modern organic electronics.

[1]Słodek, A.; Filapek, M.; Schab-Balcerzak, E.; Grucela, M.; Kotowicz, S.; Janeczek, H.; Smolarek, K.; Mackowski, S.; Malecki, J.G.; Jedrzejewska, A.; et al. Eur. J. Org. Chem. **2016**, 4020–4031.
[2]Chen, M.; Yan, L.; Zhao, Y.; Murtaza, I.; Meng, H.; Huang, W.J. Mater. Chem. C **2018**, 6, 7416–7444.
[3]Jagtap, S. *Catalysts* **2017**, *7* (9), 267–319.
[4]Bellomo, C.; Mahdi Chaari; Justo Cabrera-González; Blangetti, M.; Lombardi, C.; Deagostino, A.; Viñas, C.; Nerea Gaztelumendi; Carme Nogués; Nuñez, R.; Prandi, C. *Chem. Eur. J.* **2018**, *24* (58), 15622–15630.
[5]Chojnacka, A.; Rogalski, S.; Czapik, A.; Mieszczanin, A.; Krompiec, S.; Pietraszuk, C. *Catalysts* **2026**, *16* (3), 222–233.

MDR - D4 - P17

Polymerizations using transition metal complexes of monoanionic bidentate guanidine-ethenolate, phenolate and benzene sulfonate ligands

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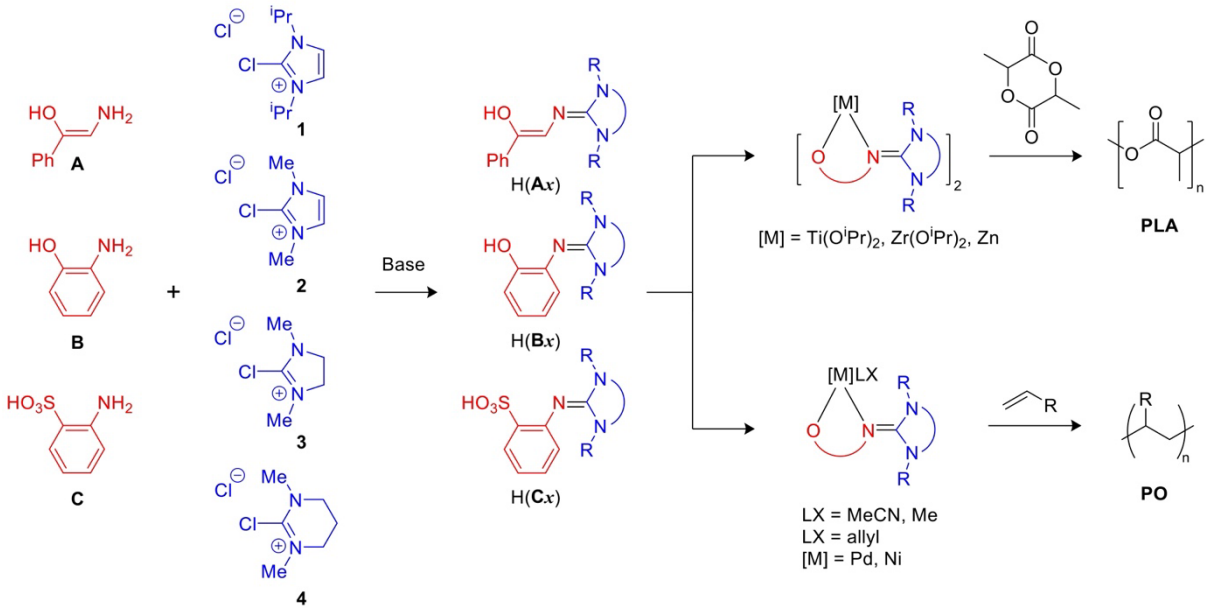
Modular guanidine-containing ligand platforms have been developed as versatile tools for controlling polymerization catalysis across multiple metal classes (see Scheme). Variations of ligand substituents enable systematic tuning of steric and electronic properties at the metal center, providing direct control over catalyst structure and, in turn, polymer microstructure and physical properties. These ligands support the ring-opening polymerization of lactide using group 12 metals, offering non-toxic alternatives to the tin-based catalysts currently employed industrially and advancing the sustainable production of biodegradable polylactide. Beyond lactide, the same ligand framework can be translated to group 4 and group 10 metals for olefin polymerization, including the challenging copolymerization of non-polar olefins with polar comonomers. This strategy establishes a unified platform for polymer synthesis, in which catalyst reactivity, selectivity, and functional group tolerance can be rationally tailored through ligand design, enabling access to both renewable polyesters and functionalized polyolefins from a common molecular toolbox.



Scheme. Guanidine-containing ligand scaffolds for the synthesis of complexes used in the polymerization of lactide and olefins.

MDR - D4 - P18
Photoinduced radical cascade for the synthesis of enantiopure 2-benzofuranyl *C*-glycosides

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Benzofurans have gained attention from chemists and biologists over the years, due to their natural occurrence in plants and wide range of biological activities such as anticancer, antiviral, antifungal, anti-inflammatory, antioxidant and so many others. Because of these properties, several synthetic strategies have been developed to synthetize benzofuran derivatives.[1,2] However, despite the importance of glycosylation to improve the the efficacy and pharmacokinetics of drugs, there are limited examples in the literature of the synthesis of *C*-glycosyl benzofuran,[3] so the discovery of new synthetic methods is of great interest.
Herein we report a mild and broadly applicable method for the construction of complex enantiopure *C*-glycosyl benzofuran derivatives through a divergent photoinduced radical cyclization cascade mechanism. Upon irradiation with visible light, spironitrochromenes **1** initiate a radical ring opening to the corresponding nitrodienes **2**, which upon radical denitrative cyclization in the presence of base, affords (1-benzofuran-2-yl)-3-deoxy-α-D-*gluco*-hex-3-enfuranoses **3**. In the absence of a base, the radical denitrative cyclization is followed by a Korblum-type oxidation to finally yield (1-benzofuran-2-yl)-3-deoxy-4-hydroxy-α-D-glucofuranoses **4**.
To sum up, this divergent approach enables the synthesis of a range of enantiopure *C*-glycosyl benzofurans that would otherwise be difficult to prepare.

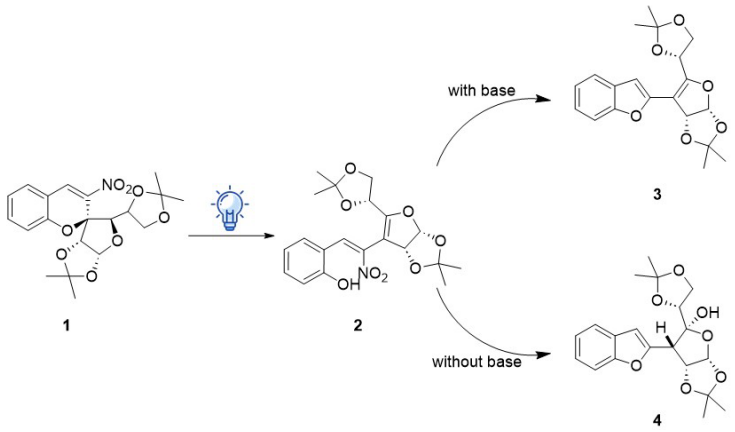

Fig. 1. Synthesis of a range of enantiopure *C*-glycosyl benzofurans.

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Funding: Patrícia I. C. Godinho thanks FCT for her PhD grant (2022.11294.BD) and P. P. R thanks University of Oviedo for a predoctoral contract (Proyecto PRP-UO-PUB-ASV-2024TESIS-23).

[1]G. Deng, M. Li, K. Yu, C. Liu, Z. Liu, S. Duan, W. Chen, X. Yang, H. Zhang, P. J. Walsh, *Angew. Chem. Int. Ed.***2019**, *58*, 2826.
[2]Kushwaha P, Chandra R. *Chem. Eur. J.* **2025**, *31*(71), e02690.
[3]Cao, Z., Zhou, X., Zhang, F., & Zhao, Y. J. Carbohydr. Chem., **2023**, *42*(4–6), 135–157.

MDR - D4 - P19
Synthesis of mevalonate derivatives via LiNTf2 catalyzed Mukaiyama Aldol reaction

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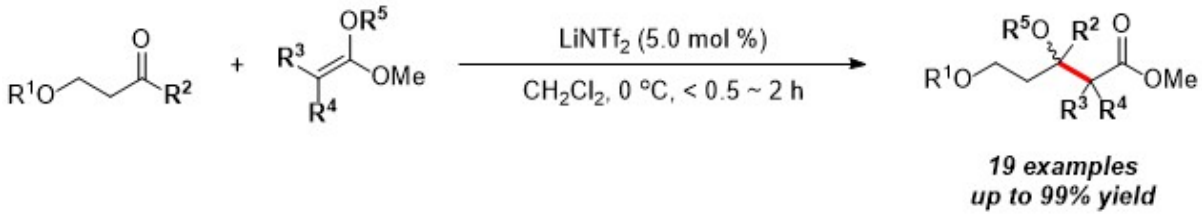
Mevalonate pathway is a critical metabolic pathway which plays a role in multiple cellular processes by synthesizing isoprenoids, such as cholesterol, vitamin K, coenzyme Q10, and steroid hormones. The substrate of mevalonate has been obtained previously through an aldol reaction of 4-hydroxy-2-butanone with benzyl acetate using LDA, which is unstable, hard to handle, and hazardous to an explosion. As an alternative, we developed a new synthetic method for the preparation of mevalonate derivatives with LiNTf2 as a catalyst of Mukaiyama aldol reaction under the mild condition. LiNTf2 is a safe, cost economy, commercially available, and efficient Lewis acid catalyst. This method is applicable to the reaction of various aliphatic substituted ketone substrates that are challenged and less reactive than aldehydes. This synthetic method has been successfully providing a wide range of tertiary β-siloxy esters with good functional group tolerance. Based on the developed method, we would like to obtain the biologically active new compounds.



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[1]H. Huang, T. Zhang, J. Sun *Angew. Chem. Int. Ed.* **2021**, *60*, 2668-2673.
[2]T. Zhang, Z. Yang, D. Zhou, F. Meng, Z. Han, H. Huang *Org. Biomol. Chem*. **2021**, *19*, 9163–6166.

MDR - D4 - P20
Mild radical construction of tricyclic tetrazoles via in situ diazotization

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Tricyclic tetrazoles are valuable heterocyclic scaffolds with significant potential in medicinal chemistry, yet efficient synthetic approaches to these frameworks remain limited. In particular, 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines have not been previously reported despite their potential bioactivity. Herein, we report a mild and efficient one-pot strategy for the synthesis of tricyclic tetrazoles via cascade diazotization and intramolecular radical C–H heteroarylation of arenes (Figure 1). Readily accessible 1-benzyloxy-5-aminotetrazoles and 1-phenethyl-5-aminotetrazoles were employed as substrates, and the reactions were conducted using sodium nitrite and acetic acid under weakly acidic conditions at room temperature. This protocol proceeds without the need for heating, catalysts, irradiation, or electrolysis, highlighting its operational simplicity. The in situ generated diazonium intermediate undergoes subsequent intramolecular radical C–H heteroarylation to afford tricyclic tetrazole products in good yields (up to 94%) without isolation of intermediates. This method enables the efficient synthesis of previously unexplored 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines as well as 5,6-dihydrotetrazolo[5,1-*a*]isoquinolines. Furthermore, bromo-substituted products were successfully diversified via Suzuki and Sonogashira cross-coupling reactions, demonstrating their synthetic utility. This study provides a straightforward and practical approach to structurally complex tetrazole-fused polycycles under mild conditions, offering new opportunities for the development of bioactive molecules.[1]

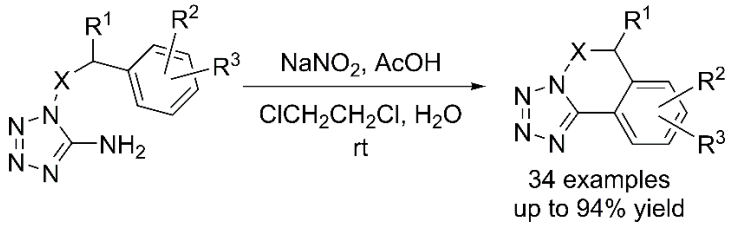

Fig. 1. Cascade diazotization/intramolecular radical C–H heteroarylation of arenes

[1]Ha, H.-J.; Kim, B.; Jo, S.; Kim, S.; Park, J.; Cho, C.-W. *J. Org. Chem.* **2023**, *88*, 2714–2725.

MDR - D4 - P21

Nazarov cyclization of α-SCF_3 Vinyl (Hetero)aryl ketones enabled by trifluoromethylthio group

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Cyclopentenone-fused polycyclic compounds are important structural motifs frequently found in natural products and pharmaceutical intermediates. Among various synthetic approaches, the Nazarov cyclization of divinyl ketones represents a powerful strategy for constructing cyclopentenone frameworks, although its application to aryl vinyl ketones remains challenging due to their low reactivity. Herein, we report a trifluoromethylthio (SCF_3)-promoted Nazarov cyclization of α-SCF_3-vinyl (hetero)aryl ketones using trifluoromethanesulfonic acid (TfOH) in dichloromethane (Figure 1). This method enables efficient access to α-SCF_3-substituted cyclopentenone-fused polycyclic compounds in good to excellent yields (up to 96%) under relatively mild conditions. The resulting bromo-substituted products can be readily diversified via Sonogashira and Suzuki cross-coupling reactions, demonstrating their synthetic versatility. Furthermore, density functional theory (DFT) calculations reveal that the α-SCF_3 substituent significantly lowers the activation barrier, thereby promoting the cyclization. This study provides a practical and efficient strategy for accessing a previously unexplored class of SCF_3-substituted polycyclic compounds with potential applications in medicinal chemistry.[1]

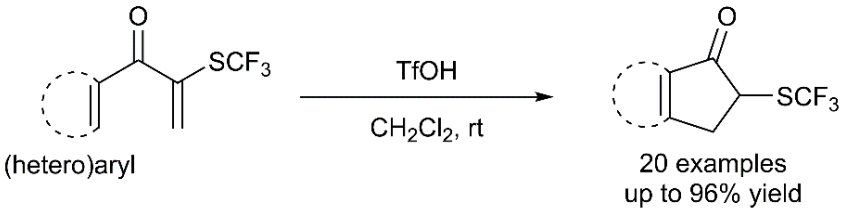

Fig. 1. SCF_3-promoted Nazarov cyclization of α-SCF_3 vinyl (hetero)aryl ketones

[1]Kim, S.; Pyo, Y. J.; Park, G. R.; Kang, H.; Ha, H.-J.; Kim, S. H.; Nam, H. Y.; Cho, D.; Cho, C.-W. *Org. Biomol. Chem.* **2026**, *24*, 360–368.