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book of abstracts

May 29th, 2026

PostgRaduatE ChemIcal SciEnces 2026 (PRECISE2026) International Conference

Book of Abstracts

May 29, 2026

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Conference Program

Faculty of Chemistry and Chemical Technology, University of Ljubljana,
Večna pot 113, SI-Ljubljana

May 29th, 2026; Lecture Hall 4

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Analytical Chemistry

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Tjaša Stopar: Chromatographic Optimization for Multi-Class Drug Determination in Hair

9.15 – 9.30
Weigeng Liu: The novel cell surface display biosensors for acetaldehyde detection

9.30 – 9.45
Demian Špaleta: Colorimetric Sensor Arrays for Non-Invasive Monitoring of Historic Paper Degradation

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Kaja Gliha: Evaluating thermal stability of choline chloride/polyalcohol deep eutectic solvents

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Sara Semeraro: Combined Use of Fourier Transform Infrared Spectroscopy and Partial Least Squares Regression for Dating Historical Parchments

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Environmental Chemistry & Water Chemistry

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11.00 – 11.15
Sonja Mavri: Comparative study of vacuum evaporation and flocculation-Fenton oxidation for treatment of oil-water emulsion waste

11.15 – 11.30
Lan Čuček Meršol: Tyre wear particles in aquatic environments: A study of interactions between microplastics from car tyres and small duckweed Lemna minor

11.30 – 11.45
Ivan Mitevski: Electrodegradation of Triton X-100: Efficacy and Transformation Products

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Vuk Martinović: Hydrophobization of nanocellulose materials with nitrogen plasma and their use in oil-water separation

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Organic Chemistry & Biochemistry

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14.15 – 14.30
Urban Barbič: SNHS Ester–Enabled Carborane Functionalization from Small Molecules to Proteins

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Plenary Lecture

Studies of Nanoporous Materials with Solid-State Nuclear Magnetic Resonance

Jakob Höfferle[1,2], Andraž Krajnc[1] and Nataša Zabukovec Logar[1,3]

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Nanoporous materials such as zeolites, metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) play a vital role in countless technologies for gas storage, separations, and catalysis, owing to their high surface areas and well-defined pore architectures. The importance of this field has been recognised by the 2025 Nobel Prize in Chemistry, awarded to Susumu Kitagawa, Richard Robson, and Omar M. Yaghi for the development of MOFs. For rational design of these materials, we need methods that can resolve local structure, defects, and host-guest interactions under realistic conditions. Solid-state nuclear magnetic resonance (ssNMR) spectroscopy is particularly powerful in this regard, as it gives site-specific information on different nuclei in both crystalline and disordered materials and complements diffraction and modelling to build an atomic-scale picture of the structure.

We will discuss defect-engineered MOFs for CO_2 capture, focusing on the amine-functionalised framework NICS-24 and its comparison to the related MOFs. A combination of multinuclear experiments, including 2D correlation techniques, is employed to probe framework environments and CO_2/H_2O binding in as-synthesised, activated and gas-loaded samples. We will then briefly turn to nanoconfined coordination-polymer glass–COF "infiltration hybrids," where multinuclear ssNMR sheds light on how melt-state glass infiltration restructures the COF pore interface and stabilises the hybrid membrane architecture. Together, these examples illustrate how ssNMR connects local structure to adsorption and transport behaviour across a diverse set of nanoporous materials.

Analytical Chemistry

Chromatographic Optimization for Multi-Class Drug Determination in Animal Hair

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Hair analysis for illicit drugs and therapeutic substances is still a major challenge, mostly due to complexity of the keratinized matrix, multiple drug incorporation pathways and scarcity of certified reference materials. In this study, three chromatographic methods performed with liquid chromatography coupled with triple quadrupole were evaluated for the determination of selected drugs and metabolites at trace levels as a preliminary step of reference materials characterization studies. Method performance was assessed in terms of linearity, sensitivity, accuracy and precision, with particular focus on the influence of chromatographic conditions such as columns and solvents, and the use of internal standards. All methods showed acceptable linearity; however, significant differences were observed in sensitivity and quantitative reliability. One of the methods demonstrated superior performance, achieving limit of detection at 0.1 pg/mg and limit of quantification at 1.0 pg/mg for all analytes. This method also showed the most consistent accuracy across concentration levels. The use of internal standards improved quantification, particularly at low concentrations, by compensating for variability related to matrix effect and ionization efficiency in electrospray ionization. These findings highlight the critical role of method optimization and internal standard selection, and establish a robust analytical framework for highly sensitive multi-class drug determination in complex matrices such as hair.

The novel cell surface display biosensors for acetaldehyde detection

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Biosensors based on cell surface display technology are among the most important detection methods. In this study, two different host strains were used to develop a sensitive, convenient, and efficient optical biosensor for acetaldehyde detection. Acetaldehyde dehydrogenase (AldH) was displayed on the surface of *Saccharomyces cerevisiae* BY4741 and *E. coli* BL21 (DE3) using flocculin protein and the N-terminal ice nucleation protein (INP), respectively. The coenzyme NAD^+ was reduced during acetaldehyde dehydrogenation, and the resulting NADH was detected by spectrophotometry. Successful construction of yeast and bacterial surface display platforms was confirmed by laser scanning confocal microscopy. The optimal AldH-display system for yeast and bacteria was identified by comparing qPCR results and whole-cell enzyme activity. Optimum reaction conditions were determined by testing temperatures from 20°C to 50°C and pH values from 5.6 to 10.6. The differences between the two display systems were compared. The highest whole-cell activities under optimal conditions were 3.68 ± 0.07 U/mL/OD_{600} for BY-S6G (yeast) and 6.95 ± 0.04 U/mL/OD_{600} for E-32-IrA (bacteria). The best-performing strains were selected for acetaldehyde detection, showing linear relationships between acetaldehyde concentrations from 0 μM to 100 μM and absorbance at 340 nm, with a limit of detection of 0.13 μM. The developed biosensors demonstrated substrate specificity and accuracy, and were successfully applied, achieving simple detection and good performance. These results indicate that AldH surface display strains have broad application potential in the field of biosensors.

Colorimetric Sensor Arrays for Non-Invasive Monitoring of Historic Paper Degradation

Demian Špaleta[1], Hend Mahgoub[2] and Matija Strlič[1,2]

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In paper conservation, oxidation and acid hydrolysis are recognized as the primary degradation mechanisms affecting the long-term stability of historic paper artefacts and are intensified under elevated temperature and high relative humidity. As degradation progresses, paper emits a complex mixture of volatile organic compounds (VOCs), including organic acids, aldehydes, alcohols, and ketones. These emissions are not only by-products of ongoing reactions but may also contribute to further deterioration. This study investigates the correlation between VOC emissions, as chemical markers of degradation, and the composition and deterioration pathways of historic paper, with particular focus on lignin-rich acidic paper due to its susceptibility to rapid ageing. A non-invasive colorimetric sensor array was developed to distinguish between alkaline printing paper and a historic book. A range of chemoresponsive colorants, immobilization strategies, and support materials were systematically evaluated. Microcrystalline cellulose (MCC) on glass and silica on aluminium (TLC plates) were assessed for their influence on sensitivity, selectivity, and stability. Hydroxyethyl cellulose (HEC) was used for dye immobilization and to enhance resistance to hydrolysis, oxidation, and photobleaching. Sensors were tested under controlled conditions and monitored using portable imaging systems. Components exhibiting rapid and reproducible colour changes were identified through multivariate analysis of imaging data and dye–analyte interaction kinetics. The resulting arrays enabled reliable classification of acidic and alkaline paper environments based on distinct colorimetric response patterns. Overall, this work demonstrates the potential of colorimetric sensor arrays as a non-invasive and cost-effective tool for characterizing and monitoring degradation processes in heritage materials.

Evaluating thermal stability of choline chloride/polyalcohol deep eutectic solvents

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Deep eutectic solvents (DESs) have emerged as promising green alternatives to conventional organic solvents, particularly for extracting bioactive compounds. Because these solvents are often exposed to elevated temperatures for extended periods during extraction processes, their thermal stability is a critical parameter. In this study, the thermal stability of three choline chloride-based DESs with polyalcohol hydrogen bond donors (1,4-butanediol, glycerol, and ethylene glycol) was systematically investigated. Both pure and diluted systems containing 25% water (w/w) were analyzed to simulate typical extraction conditions. Short-term thermal stability was evaluated using dynamic thermogravimetric analysis in the temperature range of 25 to 350 °C, while long-term stability was assessed under isothermal conditions at 60 °C and 80 °C for 2 hours. All DESs exhibited high onset degradation temperatures (>195 °C), indicating stability well above common extraction temperatures. The results showed that the type of hydrogen bond donor and water content significantly influenced thermal behavior. Long-term experiments revealed minor degradation in pure DESs, confirming that onset degradation temperatures may overestimate practical stability, while diluted systems showed greater weight losses. Nevertheless, all investigated DESs demonstrated sufficient stability under relevant isothermal conditions. These findings contribute to a better understanding of thermal behavior of DESs and support their application in green extraction techniques such as ultrasound- and microwave-assisted extraction.

Combined Use of Fourier Transform Infrared Spectroscopy and Partial Least Squares Regression for Dating Historical Parchments

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Determining the age of parchment documents is essential for assessing their authenticity, understanding the production process, and supporting conservation strategies. However, due to their historical value, the use of destructive techniques such as radiocarbon dating is not always possible. This study aimed to develop a non-invasive method for dating historical parchment using external reflectance Fourier transform infrared spectroscopy (ER-FTIR) combined with chemometric analyses. To achieve this, a dataset of 83 parchments dated between 1480 and 1965 was collected in the range 400-7500 cm^{-1}, and a subset dated between 1700 and 1900 in the range 400-1800 cm^{-1} was used to develop the model. Principal component analysis was applied to the reduced dataset to eliminate outliers, and a partial least squares regression model was developed to estimate the production date of the samples. The resulting coefficient of determination (R^2) value of 0.44 indicated a moderate predictive ability of the model, while the root mean squared error of prediction corresponded to a misdating of 51 years. These results demonstrate the potential applicability of the ER-FTIR technique for acquiring spectral data for dating historical parchments, although further improvements are required to enhance the accuracy of the proposed method.

Improving the statistical reliability of differential scanning calorimetry-based quality assessment of recycled polyethylene terephthalate

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The increasing accumulation of plastic waste has heightened the need for reliable quality assessment methods for recyclable materials such as polyethylene terephthalate (PET). Differential scanning calorimetry (DSC) is widely used to characterise the thermal properties of polymers; however, its statistical analysis is often limited by inadequate data preprocessing, which can compromise the reliability and comparability of results. This study investigates whether standardised preprocessing enhances the statistical evaluation of DSC data for recycled PET. Industrial recycled PET samples were preliminary analysed using DSC, and thermal parameters related to crystallisation, glass transition, and melting were extracted. All parameters were subjected to z-score standardisation before principal component analysis (PCA) and hierarchical cluster analysis (HCA). Standardisation reduced the dominance of high-variance variables and enabled clearer identification of relationships among parameters. PCA indicated that crystallinity is the main source of variability in the dataset, while HCA separated the samples into three distinct groups reflecting differences in crystalline and amorphous structure. The results demonstrate that appropriate data preprocessing is essential for reliable DSC-based quality assessment of recycled PET. The proposed approach improves the consistency and interpretability of the results and provides a practical framework to support recycling process optimisation. The methodology is also applicable to other polymer systems and complex material datasets.

Environmental Chemistry & Water Chemistry

Comparative study of vacuum evaporation and flocculation-Fenton oxidation for treatment of oil-water emulsion waste

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This study evaluated the effectiveness of vacuum evaporation compared to combined flocculation-Fenton oxidation for treating industrial waste emulsions, focusing on COD removal, volume reduction, and changes in water quality. Vacuum evaporation consistently achieved high COD removal (94-95%) across varying operating conditions. The process also significantly reduced waste volume (up to 85%), with optimal performance observed at 40°C and 45 mbar. COD reduction showed little dependence on treatment time, indicating rapid removal of separable contaminants. In contrast, flocculation alone achieved moderate COD reductions (45-54%), while the addition of Fenton oxidation improved performance to a maximum of 89%. Despite this improvement, the chemical treatment remained less effective than vacuum evaporation. Additionally, the process increased sample volume due to reagent addition, negatively impacting economic feasibility. Physicochemical analysis revealed further differences: vacuum evaporation produced water with low conductivity and minimal ionic content, whereas Fenton-treated samples exhibited high conductivity and elevated sulfate concentrations due to added chemicals and reaction by-products. These findings highlight the fundamental distinction between separation and reaction-based treatments. Overall, vacuum evaporation proved more efficient, simpler, and scalable, while Fenton oxidation requires careful optimization and introduces additional chemical complexity into the treated water.

Tyre wear particles in aquatic environments: A study of interactions between microplastics from car tyres and small duckweed *Lemna minor*

Lan Čuček Meršol[1], Gabriela Kalčíková[1], Barbara Klun[1] and Ula Rozman[1]

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Microplastics are a global environmental problem, because they can enter different ecosystems through a variety of sources. While the amount of microplastics in the environment is constantly increasing, it is difficult to remove them. Most types of microplastics are in the form of fragments, formed during the fragmentation of larger plastic items. Many microplastics in the environment are also tyre wear particles, generated from the abrasion of car tyres. They can be airborne or enter aquatic ecosystems as part of road dust. When they come into contact with aquatic plants, they can be adsorbed on the surface and thus enter the food chain, as plants are also a source of food to other organisms. On the other hand, adsorption can be a way to develop phytoremediation method, a method to remove microplastics from the aquatic environment. Therefore, the purpose of the research was to determine the effects of microplastics from car tyres on duckweed (*Lemna minor*), and the amount of adsorbed microplastics on the plant. Effects were evaluated by determining the specific growth rate, root length and the concentration of the photosynthetic pigments. Microplastics had no effects on the specific growth rate and on the photosynthetic pigments, while they inhibited the root length. We also found that the amount of adsorbed microplastics fluctuated during the research. The results suggest that the duckweed has the potential for phytoremediation of microplastics from car tyres, but it would be necessary to further investigate the mechanisms and the effects of environmental factors on adsorption.

Electrodegradation of Triton X-100: Efficacy and Transformation Products

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The electrooxidation (EO) of the non-ionic surfactant Triton X-100 (tert-octylphenoxy[poly(ethoxy)] ethanol, t-OPPE) was investigated as a potential approach to enhance its removal from wastewater, a significant source of environmental emissions. EO experiments were conducted in a batch reactor equipped with a boron-doped diamond (BDD) anode and a stainless steel cathode, with Na_2SO_4 employed as the supporting electrolyte. The results were evaluated in terms of degradation efficiency, reaction kinetics, and the formation of transformation products (TPs). The identification of TPs was primarily performed in sulfate media, revealing several oxidation products and indicating progressive degradation pathways, including ring-opening reactions. Particular attention was given to alkylphenols, especially 4-tert-octylphenol (t-OP), due to their toxic and xenobiotic nature. These compounds are also recognized as endocrine disruptors, exerting adverse effects on the hormonal systems of various organisms, including humans. To accurately assess the efficiency of the EO process, the development and optimization of analytical techniques for both qualitative and quantitative determination of Triton X-100 and its TPs were essential. Consequently, multiple gas chromatography (GC) and liquid chromatography (LC) methods were refined for sample analysis. Overall, the findings demonstrate that BDD-based EO represents a robust and effective method for the removal of structurally diverse organic contaminants, highlighting its potential applicability in advanced water treatment technologies.

Noble metal-doped carbon nitride photocatalyst for enhancing pollutant degradation in water under visible light illumination

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Humanity is engaged reducing harmful compounds in the environment. In the recent years the use of semiconductor photocatalysts has proven to be a useful solution. Photocatalysis uses solar energy, a cheap, abundant and clean source. Polymeric carbon nitride C3N4 has received much attention due to its thermal and chemical stability, suitable band gap (2.7 eV), environmental friendliness and undemanding synthesis. This work deals with the synthesis of layered C3N4 (g-CN) - undoped and noble metal-doped - and characterisation of each prepared photocatalyst and its activity. The molecular structure and crystallinity of photocatalysts remain unchanged when doped with silver or palladium, but their surface area increases. The rate of the charge carrier recombination is reduced in most of the doped photocatalysts compared to g-CN and absorption of light in the visible region is enhanced. We determined which oxygen species are formed. It turns out that Pd-doped photocatalysts generate more ˙OH radicals than g-CN and Ag g-CN. In contrast, the generation of ˙O2–/e– with Pd g-CN practically does not occur, the same is observed with g-CN. The generation of ˙O2–/e– is greater in Ag g-CN, especially in photocatalysts treated in hydrogen atmosphere. Most doped photocatalysts are capable of greater degradation of the pollutant (BPA) than g-CN. Doping layered carbon nitride with noble metals therefore helps to improve its photocatalytic activity.

Hydrophobization of nanocellulose materials with nitrogen plasma and their use in oil-water separation

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Oil-water separation remains an important environmental challenge, especially in oily wastewater treatment and oil-spill remediation. This study examined whether cellulose nanofibril films and aerogels could be hydrophobized by nitrogen plasma and whether this approach could support oil-water separation. Films were prepared by casting cellulose nanofibril-glycerol dispersions on silicone substrates, and aerogels were prepared by dilution, freezing, and lyophilization. The materials were treated with nitrogen plasma and characterized by water contact angle measurements, ATR-FT-IR spectroscopy, and atomic force microscopy. The practical performance of the films was tested in a model sunflower oil-water system. Nitrogen plasma treatment converted cellulose nanofibril films from hydrophilic to hydrophobic materials. This effect was observed across the tested film thicknesses and drying temperatures. The control film prepared without silicone showed clearly lower hydrophobicity than silicone-containing films. In contrast, cellulose nanofibril aerogels were not hydrophobized successfully. They remained strongly hydrophilic, rapidly absorbed water, and showed deformation during contact angle measurements. ATR-FT-IR spectra of aerogels did not show clear evidence of siloxane-related groups, and plasma treatment was limited by the thermal sensitivity of the aerogel structure. Plasma-treated films also showed improved oil uptake compared with the untreated control. These findings indicate that siloxanes are central to plasma-induced hydrophobization of cellulose nanofibril films, while the same approach is not directly transferable to cellulose nanofibril aerogels.

Organic Chemistry & Biochemistry

Ipso substitution of activated aromatic compounds using *N*-bromosuccinimide in 1,1,1,3,3,3-hexafluoroisopropanol

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Ipso substitution is a rare and unexploited reaction in synthetic organic chemistry. It is an electrophilic aromatic substitution in which the leaving group is not a hydrogen atom. In this paper, we present an *ipso* substitution reaction where a strong C–C bond is cleaved easily at room temperature. We investigated the transformations of activated aromatic compounds using *N*-bromosuccinimide (NBS) in the alternative solvent 1,1,1,3,3,3-hexafluoroisopropanol (HFIP). Reactions were carried out on a scope of various ketones and alcohols, observing the effect of different parameters: equivalents of NBS, electronic parameters, and steric hindrance of the functional group. When two or more equivalents of NBS were used, we obtained excellent yields of the *ipso*-substituted product. In some cases, the substituted fragment of the molecule was isolated, which also provided insight into the reaction pathway.

Synthesis of functionalized epoxides and ring-opening copolymerization

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Aliphatic polyethers are versatile materials extensively used in advanced and everyday applications. Their key characteristic is the presence of ether linkages in the main chain, providing specific properties, including good hydrophilicity, chain flexibility and low glass transition temperatures. Glycidyl methyl ether provides an amorphous and hydrophilic alternative to otherwise most commonly used poly(ethylene oxide), however, additional side-chain functionalities are required to further modulate properties for use in solid polymer electrolytes. To address challenges of different side reactions, a two-component organocatalytic system combining a phosphazene base *t*BuP$_2$ with the Lewis acid Et$_3$B was used. Homopolymerization of glycidyl methyl ether using this type of organocatalytic system was successful, yielding polymers with well-defined molecular weight distributions and no detectable side reactions.

Triazolium-based Iridium(I) Complex as a Catalyst for Catalytic Hydrogen/Deuterium Exchange

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Deuterium labelling has become a prominent technique for enhancing chemical and physical properties of compounds, ranging from pharmaceuticals to functional materials. Various labelling procedures have been developed and are commonly used. The most widely employed method typically falls into the category of transition-metal catalysis, where the metal centre (commonly iridium) coordinates to a functional group within the substrate facilitating the H/D exchange. The advantage of these catalysts lies in their high reactivity, chemoselectivity and the use of mild reaction conditions. Currently, the most common catalyst employed for this exchange is Kerr's catalyst, which contains an N-heterocyclic carbene (NHC) ligand. This ligand is responsible for most of the beneficial properties that this catalyst exhibits compared to other iridium catalysts. Nevertheless, further improvements such as lower catalyst loading and higher stability are always desired. For this reason, we envisaged the synthesis of an iridium complex that uses triazole-based ligands, which could provide higher stability during H/D exchange reactions. The use of triazoles also enables a modular and more atomically efficient synthesis of these ligands. We tested the synthesized complex for its activity on four compounds, that are commonly used as test substrates for H/D exchange. The results showed excellent deuterium incorporation, which could open a new field of iridium-based catalysts for deuteration.

Discovery of a Thermophilic Esterase Active on PET Degradation Intermediates

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The production of plastic waste is increasing exponentially each year and presents a serious environmental challenge. In the search for new methods to recycle plastic waste, scientists have discovered polyethylene terephthalate (PET) hydrolysing enzymes that break down polymer chains. The final products of complete PET degradation can be recycled to obtain high-value products. However, the accumulation of depolymerisation intermediates hinders this process. Due to the amorphisation of PET at higher temperatures, the identification of thermostable 2-hydroxyethyl terephthalic acid (MHET) degrading enzymes is necessary to ensure complete depolymerisation and improve terephthalic acid (TPA) yield. The aim of this study is to identify and biochemically characterise a novel thermophilic MHET-degrading esterase, and to test its functionality in a dual-enzyme system with the benchmark PET hydrolase LCC^{ICCG}. Our enzyme retains MHET hydrolysing activity at temperatures above 70 °C and improves TPA yield in combination with LCC^{ICCG} at industrially relevant substrate loadings (30 g kg^{-1}) of amorphous PET. In this study, we expanded the known diversity of MHET-degrading enzymes, facilitating future enzyme discovery and engineering.

NHS Ester–Enabled Carborane Functionalization from Small Molecules to Proteins

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Carboranes are boron-rich polyhedral clusters that possess unique chemical and thermal stability together with unique electronic properties. Carboranes are of great interest for medicinal applications through boron neutron capture therapy (BNCT) agents. BNCT shows promise as a cancer-treating method based on the cytotoxic $^{10}B(n,\alpha)^{7}Li$ reaction. In recent years many different methods were developed for introducing carboranes into biomolecules. Some approaches rely on solid-phase peptide synthesis using carborane-containing amino acids or initiation reprograming. Alternative methodologies, including transition-metal-mediated cysteine borylation and thiol-selective palladium-mediated strategies were also developed. We developed a complementary strategy targeting amine functionalities of lysine side chains of peptides. For our purpose we designed organic carborane reagents based on N-hydroxysuccinimide (NHS) esters as they are among the most widely used reagents for amine-selective modifications. We synthesized different carborane-functionalized NHS esters and demonstrated their utility in modifying small molecules, peptides and proteins, including antibodies. These constructs, integrating therapeutic antibody targeting features with boron delivery capabilities, hold promise as multimodal agents for BNCT. Importantly, bis-NHS carboranes function as bifunctional linkers, enabling both inter- and intramolecular peptide coupling. Intramolecular coupling can generate peptides bearing hydrophobic motifs, while intermolecular reactions afford higher-order assemblies.

Chemical Engineering & Material Sciences

Development of Kinetic Models for Selected Phenolic Model Compounds

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Understanding the concepts and mechanisms of phenolic compounds' oxidation is an important step in the modification and tailoring of aromatic structures. In this work, selected model compounds (vanillin, acetovanillone, catechol and resorcinol) were investigated under oxygen in alkaline conditions. The reactions were monitored over time to follow concentration changes and evaluate the influence of reaction conditions. A generalized kinetic approach considering protonated and deprotonated species was used to describe and compare the observed behavior. The results show that oxidation strongly depends on the pH and its change during the reaction. In all cases, the formation of acidic products leads to a decrease in pH, which affects both the speciation and the reactivity of the compounds. Some systems can be reasonably described by the applied kinetic model, while others show deviations, indicating that additional (presumably radical) reactions may be involved. These differences are mainly related to the structure of the compounds, which influences their susceptibility to oxidation and the formation of intermediates. Overall, the results indicate that oxidation of phenolic compounds is not governed by a single mechanism, but rather by changing conditions during the reaction, which should be considered when designing oxidation processes for phenolic materials.

Depth damage profiling in silicon substrates during focused ion beam chemical vapor deposition

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Focused Ion Beam (FIB)-assisted chemical vapor deposition (CVD) is widely used in materials science for site-specific milling, nanopatterning, and preparation of transmission electron microscopy (TEM) lamellae with nanometer precision. In dual-beam FIB-SEM instruments, both ion-beam induced deposition (IBID) and electron-beam induced deposition (EBID) can be used to deposit protective layers prior to lamella preparation. Although these processes are routinely employed, the high-energy interaction between the beam and the substrate can induce structural damage, which is a critical consideration in material characterization. This is particularly problematic for thin films, where surface-level defects or ion implantation can alter the entire material's functional properties. In contrast, such damage is often negligible for bulk materials where the affected volume is minimal relative to the whole.

In this study, the influence of beam-assisted deposition conditions on substrate damage formation was systematically investigated on silicon wafer (110). Particular attention was given to the formation of amorphous layers, defect structures, ion implantation effects, and sputtering-induced damage beneath the deposited layers. Depositions were performed using a Thermo Fisher Helios 5UC dual-beam system equipped with a Ga^+ ion source. Protective layers were deposited prior to lamella preparation using a semi-automated procedure with Thermo Fisher AutoTEM 5 software. Top-down in-situ lift-out TEM lamellae ($10 \times 2 \times 7$ μm) were cut out and thinned to electron transparency. Lamellae were analyzed using a Thermo Fisher Talos F200X G2 operated at 200 kV. Organometallic precursors, including naphthalene ($C_{10}H_8$), methylcyclopentadienyl(trimethyl)platinum ($CH_3C_5H_4$)Pt(CH_3)$_3$, and tungsten hexacarbonyl ($W(CO)_6$), were used to evaluate different surface damage profiles. We prepared three types of sample protection depositions: EBID and IBID using W, EBID and IBID using Pt, and simultaneous deposition consisting of W and C used for both EBID and IBID.

The results provide comparative insight into damage mechanisms associated with IBID and EBID deposition routes and establish guidelines for optimizing protective layer deposition during TEM sample preparation. The findings contribute toward predictive strategies for minimizing FIB-induced damage across different classes of materials.

Recycling of Li-ion batteries based on nickel manganese cobalt oxide cathodes

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The increasing deployment of lithium-ion batteries, particularly those based on lithium nickel manganese cobalt oxide (NMC) cathode materials, raises significant environmental, economic, and safety concerns related to end-of-life management. This study investigates the recycling of NMC 622 lithium-ion batteries through a combination of mechanical disassembly, material characterization, and hydrometallurgical metal recovery. Battery components were manually dismantled, dried, and separated into individual fractions. Electrode materials were characterized using a combination of scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM–EDS) to determine morphology and elemental composition, while thermogravimetric analysis coupled with mass spectroscopy (TGA–MS) was employed to evaluate thermal behavior and distinguish between organic and inorganic fractions. Hydrometallurgical processing was applied to recover Ni, Co, Mn, and Li through controlled leaching and selective precipitation. SEM–EDS results confirmed the expected composition of NMC 622 cathode material, while TGA–MS analysis revealed significant differences in thermal stability between anode and cathode materials. The hydrometallurgical process enabled successful recovery of all target metals, with results generally consistent with theoretical expectations, although some deviations were observed due to experimental limitations and process adaptations. Overall, the study demonstrates that laboratory-scale recycling of NMC-based lithium-ion batteries is technically feasible, while highlighting the importance of process optimization, safety considerations, and scalability for future industrial applications.

Electrodeposition-driven formation and strengthening of alginate hydrogels via reconstruction

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Hydrogels are three-dimensional, highly absorbent polymer networks widely used in applications ranging from drug delivery to advanced separation systems. Their performance is strongly governed by the synthesis route, which directly determines their structure and physicochemical properties. In this study, alginate-based hydrogels were fabricated via an electrodeposition approach using copper electrodes, where key parameters, including current density and deposition time, were systematically varied to control ion release and gel formation. This method enables localised and highly controlled ionic crosslinking, which is often challenging with conventional hydrogel preparation techniques. The as-deposited hydrogels were further subjected to a reconstruction process involving drying and subsequent rehydration in an ionic solution, followed by comprehensive rheological characterisation. The results demonstrate that electrodeposition enables fine-tuning of the network structure, directly influencing crosslinking density, mesh size, and overall stiffness of the gels, while reconstruction substantially enhances these properties through additional densification and crosslinking. Notably, the mechanical strength of the hydrogels increased by orders of magnitude after reconstruction, indicating a significant improvement in material robustness and structural stability. Overall, these results highlight a highly adaptable strategy for engineering hydrogels with tailored properties, demonstrating their strong potential for advanced biomedical systems and other high-performance functional materials.

EISA-synthesized Mesoporous Nb2O5–In2O3 and Nb2O5–NiO Photocatalysts

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Niobium oxides represent a highly versatile group of materials, exhibiting a wide range of interesting and adjustable physical and chemical properties. These materials possess excellent chemical stability, being resistant to acidic and oxidative environments, which makes them suitable for use under demanding reaction conditions. Niobium(V) oxide (Nb_2O_5) is particularly attractive for photocatalytic applications due to its wide band gap (3.0–3.4 eV), making it well suited for UV-driven processes.

Volatile organic compounds (VOCs) are environmental pollutants emitted from both natural and human activities. They degrade air quality by contributing to smog, ozone formation, acid rain, and climate change, and many present health risks, such as respiratory problems, neurotoxicity, and cancer. Isopropanol, a widely used solvent in paint, inks, electronics cleaning, and chemical synthesis, produces significant VOCs emissions and wastewater. Acetone is an essential solvent in plastics, pharmaceuticals, and cosmetics.

In this study, mesoporous $Nb_2O_5 - In_2O_3$ and $Nb_2O_5 - NiO$ mixed oxide materials were synthesised using the evaporation-induced self-assembly (EISA) method. The EISA method enabled the formation of an ordered mesoporous structure through the cooperative assembly of inorganic precursors and a structure-directing surfactant, followed by calcination to remove the organic template and generate well-defined porosity. In our case, Pluronic P123 was used as the surfactant, and metal chlorides ($NbCl_5$, $InCl_3$, and $NiCl_2$) were used as precursors. The synthesised composites were prepared with varying precursor compositions corresponding to 0, 25, 50, 75, and 100 at.% (Nb to In or Nb to Ni). The synthesis was carried out for 24 h under controlled conditions at 40 ° C with a continuous airflow rate of 31 mL s^{-1} and a relative humidity (RH) of 33 %, maintained using $MgCl_2$. The materials were thermally treated at 400 °C.

Characterization of the synthesized material was performed with XRD and nitrogen sorption analysis (evaluation of porosity and surface area). Photocatalytic activity was assessed via the photooxidation of isopropanol to acetone.

Nitrogen sorption analysis showed that pure Nb_2O_5 possesses a well-developed mesoporous structure and high specific surface area. Among the mixed oxides, samples containing 25 at.% indium or nickel exhibited the highest surface area and pore volume. Increasing In_2O_3 or NiO content led to structural degradation of the pore network and a marked decrease in surface area, while pure In_2O_3 and NiO were essentially non-porous.

These structural features were reflected in the photocatalytic performance: Nb_2O_5 showed the highest isopropanol-to-acetone conversion, and the 25 at.% composites performed best among the mixed oxides. Loss of mesoporosity at higher In_2O_3 or NiO loadings resulted in reduced activity, confirming that the materials' limited photocatalytic efficiency is mainly constrained by their morphological properties.

(Micro)structural and electrochemical characterization of rGO/V_2O_5 composite

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Transition metal oxides (TMOs) represent an important class of precursor materials for the synthesis of nanocomposites due to their low cost, multiple oxidation states, high stability, natural abundance and environmental compatibility. Among them, V_2O_5 has attracted particular attention because of its proven performance in electrochemical applications. Due to its relatively low electrical conductivity and limited cycling stability, the formation of composites with other materials is often pursued to enhance its performance. Therefore, this study focuses on the preparation and characterization of an rGO/V_2O_5 composite and the investigation of its electrochemical properties for potential application in battery systems. Graphene oxide (GO) paper and GO paper containing 70 wt. % V_2O_5 were prepared using vacuum filtration, followed by electrochemical reduction via chronoamperometry to obtain rGO and rGO/V_2O_5 composite papers. Detailed structural and microstructural characterization of V_2O_5, rGO and the composite was carried out using X-ray diffraction, with emphasis on crystallite size and temperature-induced phase transitions. Morphological properties were analyzed by scanning electron microscopy (SEM) and hot-stage microscopy. The results showed that the synthesized V_2O_5 exhibits low thermal expansion and nanocrystalline structure, making it suitable for nanocomposite formation. Successful synthesis of the rGO/V_2O_5 composite was confirmed by structural and morphological analyses. A battery fabricated using the prepared composite demonstrated high capacity, as evaluated by cyclic voltammetry. These findings highlight the strong relationship between structure and electrochemical performance and confirm the potential of rGO/V_2O_5 composites as promising materials for advanced battery applications.

Evaluating the Electrocatalytic Activity in Rotating Disk Electrode, Gas Diffusion Electrode, and Electrolyzer setups

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The development of efficient and scalable electrocatalysts is essential for advancing hydrogen-based energy technologies. In this work, nickel and platinum based catalysts were systematically evaluated for the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR) across three electrochemical platforms: rotating disk electrode (RDE), gas diffusion electrode (GDE), and electrolyzer setups. By maintaining consistent catalyst loadings and experimental protocols, the influence of measurement configuration on apparent catalytic performance was critically assessed.

RDE measurements revealed that both Ni/C and Pt/C catalysts exhibit activity largely independent of metal loading, reflecting intrinsic reaction kinetics under well controlled mass transport conditions. In contrast, GDE experiments showed increased variability and a stronger dependence on catalyst loading, particularly for ORR, where lower platinum loadings resulted in significantly reduced specific activity. These discrepancies are attributed to differences in catalyst layer structure, mass transport limitations, and reactant accessibility in the GDE configuration. Notably, HER activity demonstrated good agreement across RDE, GDE, and electrolyzer measurements, with consistent potentials required to achieve -10 mA cm^2, indicating that trends observed in half-cell experiments can translate to full-cell systems under certain conditions.

Overall, this study highlights that different electrochemical techniques probe distinct aspects of electrocatalyst performance. While RDE measurements provide reliable insight into intrinsic kinetics, GDE and electrolyzer setups capture additional effects related to catalyst utilization and mass transport. A combined, multi-platform approach is therefore essential for the accurate evaluation and benchmarking of electrocatalysts for practical hydrogen energy applications.

CFD Modelling OF Macro Meso Porous Monoliths in Knoevenagel Condensation Reaction

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In this study, 2D axisymmetric homogenized monolith geometry was used to develop a steady-state CFD model, which was applied to investigate the heterogeneous continuous flow catalyzed Knoevenagel condensation reaction. The CFD model encompasses convective fluid flow in the macro pores, species diffusion and chemical reaction kinetics in the meso pores of the porous monolith. The model's accuracy was acknowledged through successful validation against the previous experimental data available in the literature for the Knoevenagel condensation reaction. Subsequently, the CFD model was employed to determine the influence of key structural parameters, such as meso and macroporosity on diffusion and flow. Moreover, reaction parameters, including the temperature and multi-scale reactor size, were explored, ranging from the pore scale level to the reactor length. These CFD simulations provided an in-depth comprehension of pore flow and concentration behaviors at the macro-meso level, offering deep insights for optimizing the porous structures in hierarchical monoliths.

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