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Investigating Neo-Assyrian ceramic technology with small-angle neutron scattering

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Understanding how technologies and ideas moved between imperial centres and peripheral regions is an important topic in Near Eastern archaeology. In the Neo-Assyrian Empire (ca. 934–609 BCE), pottery was not only a practical commodity but also part of wider economic and social networks. Among the most distinctive ceramic types of this period is the fine, thin-walled pottery known as Palace Ware. Although Palace Ware has often been associated with highly standardized production in the Assyrian heartland, it is still unclear how these vessels reached provincial regions and whether they were imported, locally produced, or made by potters moving between different parts of the empire.

This project focuses on pottery from the site of Grd-i Tle in the Rania Plain of Iraqi Kurdistan, located on the eastern edge of the Neo-Assyrian Empire. Excavations have uncovered both local Iron Age pottery and examples of Palace Ware, suggesting strong connections between the site and the Assyrian core region. The main aim of the study is to identify the forming techniques used to produce these ceramics and to explore what they can reveal about the circulation of pottery, technological knowledge, and skilled craftspeople within the empire.

The research is part of an ongoing PhD project that combines several archaeometric methods. Ceramic samples are being analysed using optical petrography, X-ray fluorescence (XRF), X-ray diffraction (XRD), and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX) to investigate raw materials, provenance, and manufacturing practices.

Small Angle Neutron Scattering (SANS) will add an important new dimension to this work. SANS is a non-destructive technique that can examine the internal structure of ceramics at the nanoscale. In particular, it can detect patterns in the orientation of pores and clay particles that result from different forming methods. This is especially valuable for fine ceramics such as Palace Ware, where visible traces of manufacture are often absent or hidden by surface treatments. By analysing these internal structural patterns, SANS may help distinguish between techniques such as wheel-throwing, coil-building, and percussion-building. The project will assess the potential of SANS for identifying ceramic forming techniques and will integrate these results with compositional and petrographic data obtained through other analytical methods. By comparing Palace Ware with local pottery traditions at Grd-i Tle, the study aims to provide new evidence for discussions of technological transfer, craft specialization, and interactions between the Assyrian imperial centre and its

provincial regions. More broadly, it will explore how neutron-based methods can contribute to archaeological questions that are difficult to address through typology and visual examination alone.

Hydroxiapatite for bioapplication fields

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As life expectancy increases, the demand for biomaterials suitable for bone substitution and regeneration continues to rise. Hydroxyapatite, the primary inorganic component of bone tissue, offers significant potential due to its exceptional biocompatibility. The use of sustainable and cost-effective waste materials such as eggshells, which are composed of 91–94% calcium carbonate and contain beneficial trace elements like magnesium and strontium, has attracted considerable attention for calcium-phosphate synthesis.

In a previous study, pure hydroxyapatite was produced using a mechanochemical method with locally sourced eggshell-derived calcium oxide and diammonium hydrogen phosphate through attritor milling. A subset of the synthesized samples underwent secondary calcination at 900 °C to assess thermal effects. Structural and morphological characterizations (XRD, FTIR, SEM, EDS) indicated that the as-prepared nanocrystalline hydroxyapatite transformed into a highly crystalline hexagonal phase following heat treatment. Quantitative XRD revealed the thermal evolution of a secondary phase without decomposition of hydroxyapatite into other calcium-phosphates. SEM analysis showed a significant morphological shift from aggregated nanoparticles to well-defined larger grains, with a rough, textured surface and a macroporous network containing interconnected channels. However, complementary SANS measurements would provide valuable quantitative data on multiscale porosity and powder morphology, which are critical parameters influencing bioactivity.

EDS confirmed a Ca-P-O-rich composition. These results suggest that eggshell-derived hydroxyapatite has substantial potential for optimization in bone tissue engineering applications.

Real Time Nitrogen Management in Wheat Using Decision-Support Tools: Potential of Neutron-Based Analytical Techniques for Assessment and Validation

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Nitrogen is the most limiting nutrient in wheat production and conventional blanket fertilizer recommendations often fail to synchronize nitrogen supply with the crop's real-time demand, resulting in low nitrogen use efficiency and suboptimal yields. To address this, a field experiment was conducted during rabi (winter) season of 2023-24 and 2024-25 at the Research Farm of Sher-e-Kashmir University of Agricultural Sciences and Technology, Jammu on sandy clay loam soil characterized by slightly alkaline pH (7.46), low organic carbon (0.435 %) and available nitrogen (221.56 kg ha^{-1}) but moderate in phosphorus (15.18 kg ha^{-1}) and potassium (148.67 kg ha^{-1}). The experiment was laid out in randomized block design with three replications, comprising fourteen treatments involving conventional fertilization and real time nitrogen management strategies using Leaf Color Chart (LCC), Sufficiency Index and GreenSeeker based approaches at varying thresholds and nitrogen application rates. These treatments were designed to dynamically align nitrogen application with crop demand. Experimental results demonstrated that LCC ≤ 5 at 20 kg N ha^{-1} splits significantly enhanced growth parameters, yield attributes, grain and straw yield, total nutrient uptake which was statistically comparable to LCC ≤ 4 at 20 kg N ha^{-1}, GreenSeeker-directed N application ≤ 0.8 NDVI at 20 kg N ha^{-1} and sufficiency index-based N application ≤ 95 percent at 20 kg N ha^{-1} during both years. The superior performance of these treatments underscores the effectiveness of decision-support tools in optimizing nitrogen supply, improving nitrogen use efficiency and enhancing crop productivity.

To further strengthen nitrogen assessment and validate plant and soil elemental composition, neutron-based analytical techniques such as Neutron Activation Analysis (NAA) [1] and Prompt Gamma Activation Analysis (PGAA) can be employed as they offer high precision, multi-elemental and non-destructive quantification capabilities [2]. Integration of these techniques can provide deeper insights into nitrogen status, improve the calibration of sensor-based (SPAD meter and GreenSeeker) and visual decision support tools (LCC) and support the development of more accurate real-time nitrogen management strategies.

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Colloidal aggregation behavior

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We utilized synchrotron SAXS to explore the nanoscale aggregation behavior of single-layer bentonite colloids induced by alkaline earth metal ions. All four alkaline earth ions promote face-to-face stacking, with the aggregation capability following the order Ba^{2+} > Sr^{2+} > Ca^{2+} > Mg^{2+}. This work demonstrates that synchrotron SAXS offers unique advantages for probing colloidal structural evolution in solution environments, providing valuable methodological support and data for high-level radioactive waste (HLW) disposal safety assessments.

Neutron detectors based on boron-10

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This presentation introduces a class of neutron detectors based on thin boron-10 converter coatings, with CDT's Jalousie detector as a central example. Because neutrons do not produce an electrical signal directly, the detector first has to convert them into charged particles. In bor-10 based detectors, an incoming neutron is absorbed in a 10B4C layer, producing short-ranged charged particles that can then be measured in a gas-filled readout system. From this signal, the detector reconstructs where and when the neutron arrived.

The Jalousie design is one practical way to make this principle efficient for large-area neutron instruments. Its inclined, "Venetian-blind" converter geometry increases the neutron absorption path while keeping the detector modular and spatially precise. Starting from the basic detection physics, the talk will explain how converter thickness, geometry, gas readout, and module design influence efficiency, resolution, timing performance, and scalability. Examples from CDT detector developments for POWTEX and ESS instruments such as HEIMDAL and DREAM will show how this type of boron-based detector is adapted to demanding modern neutron scattering experiments.

Characterization studies using Small Angle Neutron Scattering for Carbon dots and Graphene oxide based Optical Biosensor

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Colloidal quantum dots (QDs) are promising materials for light emission devices (LEDs) and optically pumped lasers application, thanks to their highly tunable optoelectronic properties. As an example, CdS is a promising gain medium for OPLs, especially in the bulk nanocrystal regime [1], where the bandgap becomes independent of size. A major role on the stability of QDs in various environmental conditions, like solvent, temperature and humidity, is played by the ligands that passivate the QD. In this work, we probe the influence of ligand shells and surface coatings on optical properties of small sized quantum dots by means of combination of UV–Vis absorption, steady-state and time-resolved photoluminescence, and transient absorption spectroscopy. In addition, we will conduct small angle neutron scattering (SANS) experiments to resolve the key interphases, such as the ligand/solvent interphase, exploiting contrast variation, to correlate the surface composition and morphology with experimental optical response and theoretical predictions, paving the way to the design of a quantum dot digital twin.

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Oxidative Treatment of Ibuprofen as An Emerging Water Pollutant

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This study investigates the oxidative treatment of Ibuprofen (IP), a widely used non-steroidal anti-inflammatory drug and recognized emerging contaminant, through the application of the Fenton process. Ibuprofen frequently enters aquatic environments due to improper disposal, incomplete metabolism, and inefficiencies in conventional wastewater treatment systems, posing risks to both ecosystems and human health. Given its persistence and bioactivity, advanced oxidation processes (AOPs), particularly the Fenton reaction utilizing hydrogen peroxide (H_2O_2) as an oxidant and ferrous ions (Fe^{2+}) as a catalyst, were explored for effective degradation. The research focused on evaluating the influence of three key parameters— pH, oxidant concentration, and catalyst concentration—on the removal of Total Organic Carbon (TOC) as a proxy for organic pollutant degradation. Preliminary experiments confirmed that neither H_2O_2 nor Fe^{2+} alone could significantly reduce TOC; only their combination produced notable removal, validating the necessity of the full Fenton reagent.

Comprehensive parametric studies revealed that the optimal conditions for TOC removal occurred at pH ~3, with an oxidant-to- catalyst (ox/cat) ratio of approximately 15, specifically at [Fe^{2+}] = 0.078 mM and [H_2O_2] = 1.18 mM. Under these conditions, 80.4% of the TOC was removed within 24 hours. These results align well with previous studies on the Fenton treatment of other contaminants, though variation is expected due to differences in pollutant structure and reactivity.

Reactor Thermal Validation – EVEREST Project at Budapest Research Reactor

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The EVEREST (Experiments for Validation and Enhancement of the REactor preSsure vessel fluence assessmenT) project focuses on improving the safety and reliability of nuclear reactors through advanced experimental measurements and modelling techniques. A key objective of the project is the analysis and validation of reactor temperature distribution during reactor start-up.

The work involved the collection, processing, and organization of temperature measurement data obtained from installed thermocouples. The recorded data were structured and stored in CSV format to support further analysis and validation activities. In addition, experience was gained in the use of the SpecView SCADA software environment, including system monitoring, data handling, and operational familiarization.

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True and Random Coincidence Summing Effects at HPGe Detector Systems

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We were quantitively investigating true and random coincidence summing effects of a Eu-152 source measured with the multiplex detector system FIPPS at the ILL as well as two HPGe detectors at the FRM II in Garching. In theory a coincidence peak area can be computed from the activity of the source, the partial gamma emission probabilities of the coinciding gammas, and the detector efficiency for the corresponding gamma energies. Using the gamma spectrum evaluation program Hypermet and the graphical interface Cubix, which is employed at the ILL, the single gamma as well as coincidence spectra were analysed and compared to the theory. Additionally, spectra of measurements performed with single detectors were evaluated to determine the discrepancy of the coincidence summing equations for one and multiple detectors.

Gold Nanoparticles and Nanoscale Heterogeneity in Qing Dynasty Rose Enamels: Exploring the Potential of Neutron Scattering for Au° Nanoparticle Characterization

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Famille rose enamels represent one of the most significant technological innovations in Qing dynasty porcelain production. Their characteristic pink coloration arises from a dispersion of metallic gold nanoparticles (0.1 %wt) within a lead-rich glass matrix, producing color through plasmonic interactions [1]. However, the nanoscale structure of these particles and their relationship to color formation remain incompletely understood.

Preliminary non-invasive investigations of gold-containing rose enamels from Qing dynasty porcelains using Raman spectroscopy reveal intense luminescence and characteristic low-wavenumber Raman signals, while XRF measurements confirm the occurrence of gold in rose-colored regions. However, visually distinct rose and pale-pink regions exhibit different Raman/luminescence and XRF responses despite belonging to the same decorative system, suggesting variations in nanoparticle concentration, aggregation state, or spatial distribution at the nanoscale.

To further investigate these nanoscale differences, the present program seeks to explore the potential of small angle scattering techniques for the characterization of historical enamel materials. Recent studies have demonstrated that Small-Angle X-ray Scattering (SAXS), particularly when combined with Transmission Electron Microscopy (TEM), can characterize the size and size distribution of gold nanoparticles in inorganic matrix [2,3]. Such approaches suggest a promising pathway for investigating nanoscale heterogeneity in gold-bearing rose enamels. A key preliminary step would be to evaluate whether SAXS can detect gold-related scattering signals from powdered rose enamel through comparison with colorless glaze. Establishing the detectability of these signals would provide an essential feasibility assessment for future scattering studies of historical enamels. If successful, the results could serve as a basis for evaluating the applicability of neutron-based techniques, including Small-Angle Neutron Scattering (SANS), to the investigation of gold nanoparticle distributions in ceramic enamels.

By combining Raman and luminescence spectroscopy, XRF analysis, and advanced scattering approaches, future research may help characterize the distribution and organization of gold nanoparticles within historical enamel layers. More broadly, this work seeks to evaluate the potential contribution of scattering techniques to the study of historical glasses, enamels, and ceramic technologies

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Operando Neutron Reflectometry Study of Stack Pressure Effects on Interface Evolution in Anode-Free Solid-State Batteries

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Anode-free solid-state batteries offer a promising route to maximise energy density by eliminating the pre-lithiated anode. However, their performance is fundamentally limited by unstable lithium plating/stripping behaviour and loss of electro-mechanical contact at the copper current collector. Recent work highlights that these degradation processes arise from coupled electro-chemo-mechanical effects, where interfacial stress evolution and lithium morphology are strongly interdependent [1]. Among key operational parameters, stack pressure plays a critical role in governing interfacial contact stability and electrochemical performance in solid-state systems [2]. However, its direct impact on the buried interface structure during operation remains unresolved.

As part of an upcoming Master's thesis project, this work proposes an operando neutron reflectometry (NR) study to investigate the role of stack pressure on interfacial evolution in anode-free solid-state thin film cells. NR enables non-destructive, depth-resolved probing of buried interfaces and is uniquely sensitive to lithium, allowing quantification of layer thickness, roughness, and scattering length density during electrochemical cycling [3]. Specifically, the structural evolution of the buried interface is resolvable due to the inherent neutron scattering length density contrast between the solid electrolyte and electrodeposited metallic lithium.

To investigate these interfacial dynamics, the proposed experimental design utilises a thin film model cell consisting of a silicon substrate serving as a neutron transparent beam entry window, followed by a sputtered Cu current collector layer (10-30 nm), a LiPON solid electrolyte (200-300 nm), and a $LiCoO_2$ cathode. Lithium is electrodeposited in situ at the buried Cu/LiPON interface during the first charge. Cells are assembled under controlled stack pressure (0.1, 0.5, and 1.0 MPa) using spring-loaded fixtures to maintain constant pressure throughout cycling.

The central research question is whether increased stack pressure promotes the formation of dense, stable lithium deposition with reduced void formation at Li/LiPON interface or accelerates mechanical degradation and interfacial contact loss. Operando NR measurements are correlated with electrochemical impedance spectroscopy (EIS) to link structural evolution with interfacial resistance changes.

This study aims to provide a depth-resolved mechanistic insight into pressure-dependent interfacial evolution in model systems, with implications for the design of mechanically stable, high-energy-density anode-free solid-state batteries.

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The Water-Wire Hypothesis for Tryptamine Functional Selectivity

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Positional isomers of methoxy-substituted tryptamines exhibit dramatically different pharmacological profiles at 5-HT2A receptors despite similar binding affinities. Structural studies reveal that tryptamines bind with their indole ring deep in the receptor's hydrophobic 'π-cage' formed by 3 residues with aromatic ring sidechains (W336/F339/F340) while the protonated tertiary amine forms a salt bridge with D1553.32, near the extracellular interface. This project investigates whether substituent-induced changes in ligand orientation alter water network organization around the amine-aspartate salt bridge, affecting proton dynamics required for receptor activation. Kinetic isotope effects (KIE) in D_2O will help reveal the degree to which proton tunnelling correlates with activity and possibly selectivity. The approach involves use of implicit and explicit solvation by density functional theory (DFT) methods, in addition to quantum-mechanics/al molecular-mechanics/al (QM/MM) calculations, towards resolving the proton transfer pathway, while additionally predicting KIE values. Sequential deuteration will pinpoint which protons are mechanistically relevant. Empirical measurements and determinations will be employed, else data-mining undertaken, where possible towards formulation of a synergy between experiment and computation.

Hypothesis: Substitutions at the 4, 5, and 6 positions of tryptamines affect their orientation within the 5-HT2A receptor's hydrophobic π-cage (W336/F339/F340). This orientation determines the positioning of the protonated tertiary amine relative to D1553.32 and the surrounding water network at the extracellular interface. Active compounds (DMT, 5-MeO-DMT) adopt orientations where the amine-Asp salt-bridge geometry permits water-mediated proton dynamics required for receptor activation. Inactive compounds (6-MeO-DMT) adopt orientations that disrupt this geometry, altering proton dynamics and preventing activation.

Molecular aggregation in aqueous solutions of 2-(diethylamino)ethanol inferred from viscosity and confirmed by the SANS experiment

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Recommended viscosity models are not suitable for associated liquid mixtures, especially aqueous solutions [1]. We extended a two-parameter model [2] to systems in which both components form intermolecular hydrogen bonds, thereby allowing self- and cross-association effects to be clearly distinguished. The model's wide applicability was confirmed by analysing 600 datasets for 150 binary systems at various temperatures and pressures. For example, viscosity data for 2-(diethylamino)ethanol (DEAE) mixtures indicated stronger cross-association with water than with methanol.

To verify these macroscopic findings at the molecular scale, small-angle neutron scattering (SANS) was performed on two binary systems containing DEAE: nine mixtures with heavy water (D_2O), at a temperature of 298.15 K and 333.15 K, and four with heavy methanol (CD_3OD) at a temperature of 298.15 K. Concentrations were up to 0.3 mole fraction of DEAE.

Aqueous solutions of DEAE showed long-range molecular ordering, similar to that in such solutions of certain cyclic [3,4] and linear amines. The Ornstein-Zernike model for concentration fluctuations well approximated the scattering curves for dilute solutions, whereas the scattering in solutions with the DEAE mole fraction of 0.15 or higher required the Teubner-Strey model with two characteristic lengths for proper interpolation. Indeed, the emerging structure is partly reminiscent of that of microemulsion, characteristic of ternary mixtures with surfactants, in the manner that an interference peak appears in the low-angle region of the neutron diffraction pattern. However, the structure evidently differs from that of the microemulsion, in which the apolar, oily phase is separated from the bulk polar water by the layer of the amphiphilic molecules. Computer simulations suggested a mechanism for the self-segregation of propylamine due to the strong water-nitrogen interactions [5]. Unlike aqueous solutions, the mixtures with heavy methanol proved to be homogeneous, which indirectly confirms the role of water as an active solvent promoting the molecular aggregation.

Preliminary results of the quantum chemical DFT calculations at the B3LYP-D3(BJ)/def2-TZVP level of theory are consistent with the conclusions drawn from the experimental data.

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Automated sample changer for the Neutron Activation Analysis laboratory at Budapest Neutron Centre

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The Budapest Neutron Centre operates 16 large-scale neutron user facilities associated with the Budapest Research Reactor. One of the reactor's oldest applications is neutron activation analysis (NAA). To facilitate the work carried out in the NAA laboratory, we implemented an automated sample changer, which was designed, built, programmed and installed lately.

At the NAA laboratory, we perform gamma spectroscopic measurements following reactor irradiation of the samples. Two high-purity HPGe detectors are used for this purpose, which are housed in two low-background chambers. These low-background chambers are special custom-built cabinets, so commercial sample changers available for HPGe detectors manufactured by Canberra or Ortec cannot be applied. The in-house-built sample changer enables automated handling and measurement of prepared sample batches, significantly improving workflow consistency and throughput by allowing up to 19 samples to be measured without operator intervention. The new setup reduces manual workload while enhancing measurement reproducibility and laboratory efficiency. In addition, the automation contributes to improved radiation safety by minimizing direct handling during operation.

The developed system represents an important modernization step for the NAA laboratory at BNC and demonstrates the benefits of automation in neutron-based analytical facilities.

Comparative structural and phase analysis of promising multifunctional nanocomposites for environmental remediation and electrical energy storage by Mössbauer spectroscopy and complementary techniques

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Rare-earth-doped goethite nanocomposites are promising multifunctional materials for applications in electrical energy storage primarily like Na-ion battery anodes and visible-light-driven water purification. We examined the phase composition of Eu-doped $Eu_xFe_{100-x}OOH$ samples synthesized by hydrothermal routes with different Eu contents (x = 0, 10, 20, 30, 40, and 50 mol%) in both the as-prepared and heat-treated states (300 °C, 30 min), as well as the structural changes induced by heat treatment, using ^{151}Eu and ^{57}Fe Mössbauer spectroscopy and powder X-ray diffraction, with particular attention to possible differences between samples prepared from Eu_2O_3 and $Eu(NO_3)_3$ precursors.

The as-prepared and heat-treated $Eu_xFe_{100-x}OOH$ composite systems derived from Eu_2O_3 and $Eu(NO_3)_3$ precursors showed distinct Eu-containing phases. XRD revealed $Eu(OH)_3$ as the principal crystalline phase in all samples, together with a considerable amorphous contribution. A pronounced precursor dependence was observed upon heat treatment: the Eu_2O_3-derived samples underwent complete transformation of goethite into hematite, whereas only partial transformation occurred in the $Eu(NO_3)_3$-derived systems. The latter retained fully antiferromagnetic goethite, while the former contained a paramagnetic component beside the antiferromagnetic component, indicating that the europium precursor significantly affects both the phase composition and the thermal phase transformation. The $Eu_{10}Fe_{90}OOH$ composite prepared from the Eu_2O_3 precursor exhibited anomalous changes in the goethite-related XRD reflections relative to the undoped sample. These changes may be attributed to Eu incorporation into the goethite structure.

The ^{151}Eu Mössbauer spectra of the 10 mol% Eu samples revealed pronounced differences in the average hyperfine parameters between the as-prepared and heat-treated states for both the oxide- and nitrate-derived systems, which are interpreted in terms of europium incorporation into the goethite. In addition, ^{151}Eu Mössbauer spectroscopy clearly confirmed that europium is present exclusively in the Eu^{3+} oxidation state in the hydrothermally synthesized systems.

The anticipated results contribute to a deeper understanding of local structural phenomena and magnetic coupling mechanisms in complex multifunctional nanocomposite systems, thereby supporting the development of advanced materials with improved environmental and energy-storage functionalities.

Spacer-length effects on the self-assembly of urea-based gemini surfactants and their templating of ordered mesoporous silica

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Urea-based cationic gemini surfactants containing polymethylene spacers with two to ten methylene groups were studied to clarify how spacer length affects their micellar self-assembly and their performance as structure-directing agents for mesoporous silica nanoparticles. The micellar systems were examined by small-angle neutron scattering (SANS) using multi-model form-factor analysis based on a core–shell ellipsoid and two homogeneous ellipsoid models [1]. The different models consistently revealed a pronounced spacer-length dependence of micellar dimensions, aggregation number, and hydration. Among the investigated surfactants, the compound containing four methylene groups in the spacer produced the largest micelles and the highest aggregation number. From U4 to U10, both micellar size and aggregation number gradually decreased. Increasing spacer length was also accompanied by a systematic reduction in shell hydration, consistent with the greater hydrophobicity of the headgroup–spacer region. Intermicellar interactions were described using the rescaled mean spherical approximation (RMSA) for screened Coulomb repulsion. U4 displayed the strongest interaction peak together with the largest separation between neighboring micelles. The same series of gemini surfactants was subsequently employed as structure-directing agents in the preparation of mesoporous silica nanoparticles through a sol–gel process under basic conditions [2]. Spacer-dependent variations in particle morphology and pore organization were investigated by nitrogen porosimetry, small-angle X-ray scattering (SAXS), ultra-small-angle neutron scattering (USANS), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Depending on spacer length,

different proportions of spherical and cylindrical nanoparticles were observed. Materials templated by U4–U10 exhibited the conventional two-dimensional hexagonal pore arrangement characteristic of MCM-41, while the sample prepared using the shortest-spacer surfactant contained two distinct crystalline structures. Spacer length further affected both the lattice spacing and the dimensions of the ordered domains. TEM measurements indicated approximately 10–20% variation in lattice spacing among individual crystalline domains. Analysis of SAXS peak broadening indicated that finite domain size was the principal source of peak broadening, whereas variations in lattice spacing made a smaller contribution.

Although spacer length produced substantial changes in micellar structure, a direct relationship between micelle dimensions or shape and the resulting silica pore dimensions was not observed. Notably, surfactants showing comparatively weak intermicellar interactions, especially those with the shortest and longest spacers, tended to generate predominantly spherical silica particles. This observation suggests that intermicellar interactions may contribute to controlling particle morphology, although the trend was not consistent throughout the full surfactant series. Overall, these findings demonstrate how spacer-controlled molecular architecture influences gemini surfactant self-assembly and, in turn, the structural characteristics of the mesoporous silica materials formed using these surfactants.

Acknowledgements

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Multiscale Characterization of Calcium- and Magnesium-Induced DNA Structural Modulation

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Calf thymus DNA (ctDNA) was used as a model polyelectrolyte biomacromolecule to investigate structural effects induced by biologically relevant divalent cations Ca^{2+} and Mg^{2+} in aqueous solution. These ions are known to influence DNA hydration, electrostatic interactions and structural properties through interactions with phosphate groups and groove-associated binding sites [1]. Understanding ion-mediated effects in hydrated DNA systems is important for the interpretation of biomolecular organization at mesoscopic length scales and for the design of future neutron scattering experiments [2].

In this work, Ca^{2+}- and Mg^{2+}-modified ctDNA systems are being investigated using complementary physical methods. UV-VIS spectrophotometry is employed to monitor changes in the DNA absorption band near 260 nm, while circular dichroism spectroscopy is used to evaluate possible effects on the characteristic B-DNA spectral profile. Dynamic light scattering and zeta potential measurements are further applied to examine possible ion-induced changes in hydrodynamic size, colloidal stability and electrostatic properties of the DNA systems. Preliminary isothermal titration calorimetry measurements are also being explored to assess weak thermal responses accompanying cation–DNA interactions.

Initial spectroscopic measurements indicate small differences in the optical response of ctDNA solutions after addition of divalent cations, while the overall spectral characteristics of native DNA remain preserved. The presented preliminary multitechnique characterization is intended to provide a basis for future small-angle neutron scattering studies of mesoscale structural organization in ion-modulated DNA systems.

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Neutron Imaging and Diffraction for Multiscale Characterization of Corrosion in Archaeological Iron Artifacts

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Iron artifacts are highly susceptible to corrosion, and understanding the distribution, composition, and structure of corrosion products is essential for their conservation. However, conventional X-ray-based techniques may have limitations in non-destructively probing corrosion products within the interior of iron artifacts. In this study, iron specimens recovered from the "Nanao No. 1" shipwreck were investigated using complementary neutron and X-ray techniques. X-ray fluorescence and μ-Raman spectroscopy were first employed to characterize the elemental composition and layered structure of the corrosion products. Combined with μ-X-ray diffraction and neutron diffraction, these analyses identified goethite and magnetite as the two major corrosion phases. The results revealed a distinct spatial distribution pattern, with goethite preferentially enriched toward the outer corrosion region and magnetite predominantly distributed toward the inner region. Neutron imaging further revealed corresponding differences in image contrast between the two phases. The contrast was associated with their different chemical compositions, particularly the hydrogen content of goethite and its strong interaction with neutrons. By integrating phase information from μ-X-ray diffraction with neutron tomography, image segmentation was performed to visualize the three-dimensional spatial distribution of the major corrosion phases within the specimens. Monte Carlo simulations were further conducted to investigate neutron attenuation in goethite- and magnetite-rich materials. The simulations demonstrated that neutron scattering and sample geometry can affect the apparent attenuation coefficient, while simulations using the experimental polychromatic neutron spectrum revealed spectral hardening and the corresponding attenuation behavior of the two corrosion phases. The combined experimental and simulation results provide a non-destructive, multi-scale approach for characterizing the internal corrosion structure of archaeological iron artifacts and improving the interpretation of neutron imaging data.

Vacuum-Thermal Exfoliation of Graphene Oxide–Boric Acid (GO–BA) Complexes and Phase Transformation of Obtained Composites in the Temperature Range of 100–1500°C

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Composites obtained from the Graphene Oxide-Boric Acid (GO–BA) system have a wide range of applications, including supercapacitors, batteries, sensors and membrane fabrication, spintronics, wastewater treatment, biomedicine, fire-resistant coatings, and the development of flame-retardant composites and etc. BA forms B–O–C linkages between graphene oxide layers, resulting in the formation of three-dimensional (3D) structured composites characterized by high mechanical strength and enhanced adhesion properties [1]. It has been established that mixing a GO suspension with an aqueous solution of BA at room temperature induces intermolecular interactions between the components, leading to an increase in the hydrodynamic diameter of GO from 250–400 nm to 600–700 nm. The concentration of BA was maintained within the range of 5–20 wt.% relative to the mass of GO. The ζ-potential of particles in the GO suspension was found to be −58 to −61 mV, whereas in the GO–BA suspension it decreased to −43 to −46 mV. In many cases, for the fabrication of specific types of materials, it is preferable to prepare graphene oxide–boron compound composites in the form of ultradispersed powders rather than films. Powdered rGO–HBO_2 composites were obtained from elastic GO–BA films by their vacuum-thermal exfoliation at 160 °C. At the same temperature, under either an inert atmosphere or in air, the films retain their geometric shape without noticeable deformation. As a result of exfoliation, the mass loss of the films reached 44–48%. The particle size of the resulting powder ranged from 1370 to 1547 nm, while the ζ-potential values were between −20 and −21 mV. In contrast, vacuum-thermally exfoliated GO samples exhibited particle sizes 768–788 nm and ζ-potential values −37 to −38 mV. GO-BA complexses undergo the following transformations with increasing temperature: GO–BA → rGO–HBO_2 (160°C) → rGO–B_2O_3 (300-500°C) → G–B_2O_3–B_4C (1500°C). The phase transformation scheme was established based on XRD analysis.

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Neutron techniques for the characterization and scale-up of chemical reactors

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Chemical reactors are widely used in the chemical industry for mass production, especially those handling multiphase flows, such as mixtures of gases, liquids, or solid particles. Characterizing these reactors is fundamental for their design, optimization, scale-up, and selection of operating conditions, and for this purpose, experimental techniques combined with numerical methods are frequently employed. The use of neutron techniques represents an innovative, non-intrusive, and non-destructive experimental approach to determining the distribution of the multiple phases coexisting within the reactor under different conditions, or to monitor the evolution of the internal process through neutron imaging and instantaneous gamma activation analysis. Furthermore, this type of experimental characterization can be used as a source of validation data for numerical models, which together, can be used for process scale-up. Small-scale reactors can be placed in the neutron beam to obtain a time-averaged phase distribution using neutron imaging, or a time-evolution of the process using instantaneous gamma activation analysis. This methodology can be applied to batch reactors, such as stirred tanks or bubble columns, or to continuous operation reactors, such as tubular reactors equipped with inserts, for the characterization and development of industrial processes in the field of CO_2 absorption, the production of critical raw materials and hydrogen generation.

Ferroelectric nematic phase at a photosensitive polymer substrate: comparing thermo-mechanical effect with photo-reorientation

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The average direction of the molecules (director) of nematic liquid crystals (LCs) can be easily oriented by light using photosensitive surfaces (photoalignment). Recently, it was shown that in polar nematic (N_F) liquid crystals the director field can be manipulated by a laser light induced temperature gradient. Here we investigate how the photoalignment compares to the thermo-mechanical effect in the N_F phase. For that we study photo-reorientation phenomena on a photosensitive polymer substrate in the prototype ferroelectric nematic liquid crystal compound DIO. It is found that, while in the nonpolar nematic and antiferroelectric mesophases the photoalignment is observed, in the ferroelectric nematic phase the thermo-mechanical (TM) coupling determines the director alignment

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Development and Characterization of the ARMAN Neutron Reflectometer at the WWR-K Research Reactor

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Neutron reflectometry is a powerful non-destructive technique for studying the depth structure of thin films, multilayers and interfaces on the nanometer scale. My PhD research is focused on the development, commissioning and experimental characterization of the ARMAN neutron reflectometer at the WWR-K research reactor of the Institute of Nuclear Physics in Almaty, Kazakhstan. The creation of this instrument is an important step toward expanding neutron scattering capabilities in Kazakhstan and enabling local studies of planar nanostructures and multilayer systems.

The ARMAN reflectometer is designed as a constant-wavelength instrument based on a double-crystal graphite monochromator, a collimation system, a sample positioning unit and a neutron detection system. During the commissioning stage, the main experimental tasks include selection and verification of the working neutron wavelength, adjustment of the beam geometry, estimation of angular divergence, optimization of the shielding configuration and testing of the instrument using reference thin-film samples.

Initial measurements on Ni/Si structures demonstrated the possibility of recording specular neutron reflectivity curves with characteristic features such as the critical edge and Kiessig oscillations. These results confirm the practical applicability of the instrument for thin-film studies and provide a basis for further development of the measurement procedure, data treatment and instrument characterization.

Current work is focused on improving the neutron-optical layout, refining the collimation and alignment procedures, increasing the quality of the measured reflectivity curves and extending the experimental capabilities of the instrument. Monte Carlo simulations using VITESS are also applied to support the interpretation of experimental results and to evaluate possible configurations of the beamline. Further development of the instrument may include an upgrade toward polarized neutron reflectometry using supermirror-based polarizing elements and spin manipulation devices.

Participation in CETS would be highly valuable for this project, since the school combines theoretical lectures on neutron techniques with hands-on practice at operating neutron instruments. In particular, deeper understanding of neutron reflectometry, beamline optimization, data treatment and comparison with other neutron methods would directly support the further development of the ARMAN reflectometer and its future application to thin-film and multilayer studies.

Multiscale Characterization of Protein–Electroactive Interfaces by Neutron Scattering

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The progressive increase in human longevity has intensified the need for strategies that extend healthspan alongside lifespan. Tissue engineering offers a promising approach through biomaterial-based scaffolds that recreate physiologically active microenvironments for tissue regeneration. In recent years, electroactive biomaterials have attracted considerable attention due to their ability to provide dynamic electrical cues that influence biological processes. Despite extensive evidence of their impact on cellular behavior, the mechanisms governing protein adsorption and organization at electroactive biointerfaces remain poorly understood. Our previous research focused on elucidating how piezoelectric and magnetoelectric biomaterials regulate protein–surface interactions and subsequently affect cellular responses. Using poly(vinylidene fluoride) (PVDF) and PVDF-based nanocomposites as model electroactive systems, it is demonstrated that surface polarization modulates protein adsorption kinetics, conformation, and interaction strength, resulting in significant differences in mesenchymal stem cell spreading and focal adhesion formation. To achieve this result, neutron scattering techniques played a crucial role, in particular:

• Neutron Reflectometry: NR was employed to investigate the structure of protein layers adsorbed on electroactive PVDF ultrathin films. Through contrast variation measurements, NR enabled the determination of the thickness, density, roughness, solvent content, and interfacial organization of collagen and fibronectin layers with nanometer resolution. The results revealed distinct adsorption mechanisms for both proteins, including the formation of highly hydrated interfacial layers and partial protein penetration into the polymer matrix, demonstrating the ability of electroactive surfaces to modulate protein organization at the nanoscale.

•Small Angle Neutron Scattering: SANS was used to characterize the nanostructure of magnetoelectric PVDF nanocomposites containing magnetic nanofillers. The technique provided information on aggregate morphology, fractal organization, and filler–polymer interactions over length scales ranging from a few nanometers to hundreds of nanometers. Analysis of the scattering profiles revealed correlations between nanofiller surface characteristics, aggregate organization, and the formation of the electroactive β-phase of PVDF, establishing structure–property relationships

that govern the macroscopic piezoelectric and magnetoelectric performance of the composites.

• Quasielastic Neutron Scattering: QENS measurements were conducted on collagen in solution to characterize their molecular dynamics and hydration behavior at pico- to nanosecond timescales.

These studies provide a reference framework for understanding protein mobility before surface adsorption.

Building on previous studies, the next steps focus on electroactive biointerfaces by linking material structure, surface polarization, and protein behavior across multiple scales. It develops piezoelectric, piezoionic, and magnetoelectric systems to control protein adsorption and enable biosensing and real-time monitoring. These materials will be engineered as biostable and biodegradable platforms ranging from scaffolds to microscale sensors and actuators, with integration into organ-on-a-chip devices for controlled stimulation and analysis of biological environments. Complementary neutron techniques will provide multiscale insight: NR for protein structure and hydration at electroactive interfaces, SANS for nanostructure–property correlations in electroactive materials, and QENS for protein dynamics in solution and in adsorbed states under surface polarization.

Structural and functional plasticity of photosystem II

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Photosystem II (PSII) is a multi-subunit protein complex embedded in the thylakoid membranes of oxygenic photosynthetic organisms. This critical complex functions as a water-plastoquinone oxidoreductase, using excitations from absorbed photons as a driving force. Traditionally PSII reaction centers are thought to possess open (PSIIO) and closed states (PSIIC) leading to minimal and maximal fluorescence (F0, FM) respectively. Recent findings regarding the light-adapted charge-separated state (PSIIL) suggest that conformational changes and dark-reversible reorganizations occur within the PSII core complex [1]. These findings challenge the traditional model by attributing FM to PSIIL rather than PSIIC.

PSII and type II bacterial reaction centers (bRC) share a common evolutionary origin and the basic electron transport reactions are similar. Our aim is to study if there is light-adapted charge-separated state also in bRC and does it also have an influence on fluorescence induction as in PSII. We have been able to show that to reach FM, multiple single turnover saturating flashes are needed. A waiting time between the flashes is also needed before the higher fluorescence level can be reached. Similar mechanisms have earlier been identified in PSII core complexes and in thylakoids [2]. The structure of bRC is less complex compared to PSII. Therefore, the changes can be more easily identified first in bRC and later in PSII.

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Structure-Property Correlation in MXene/CNT/WO_3 Hybrid Cathodes for Rechargeable Zinc–Air Batteries

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A rechargeable zinc-air battery (ZABs) has attracted significant attention as next-generation energy-storage systems owing to their high energy density and environmental sustainability. The optimized MXene/CNT/WO_3 (MCW-111) heterostructure exhibits a highly interconnected conductive framework, where $Ti_3C_2T_x$ MXene nanosheets provide rapid electron transport pathways and functionalized carbon nanotubes suppress MXene restacking and enhance electrolyte accessibility. The WO_3 nanoparticles were introducing catalytically active centers for oxygen electrocatalysis [1,2]. In rechargeable ZABs, the synergistic integration of these components results in improved oxygen reduction and evolution reaction kinetics, low charge-transfer resistance, high power density, higher specific capacity, and long-term cycling stability more than 540 charge-discharge cycles.

Comprehensive structural and electrochemical investigations reveal a direct correlation between heterointerface formation, defect-rich WO_3 domains, and improved electrochemical activity. XPS analysis indicates the co-existence of W^{6+}/W^{5+} species and, suggesting the presence of oxygen-vacancy-rich regions that facilitate oxygen adsorption, intermediate stabilization, and charge-transfer processes [3,4]. The optimized electrode architecture further promotes efficient OH^- transport through interconnected ion-diffusion pathways while maintaining structural integrity during prolonged cycling. Consequently, these structural features collectively contribute to improved reaction reversibility, reduced polarization losses, and enhanced bifunctional catalytic activity. In rechargeable zinc-air batteries, the optimized MCW-111 electrode showed excellent bifunctional oxygen electrocatalytic activity with a limiting current density of 5.7 $mA{\cdot}cm^{-2}$, a low bifunctional gap (ΔE) of 0.71 V, a high specific capacity of 737.19 $mAh{\cdot}g^{-1}Zn$, a peak power density of 80 $mW{\cdot}cm^{-2}$, and outstanding cycling stability of 540 cycles (180 hours). Future investigations using neutron diffraction and advanced structural modelling will focus on elucidating oxygen-vacancy defects and heterointerface structures in MCW-111, helps in the development of efficient metal-air battery electrodes.

The logical design of next-generation defect-engineered cathodes for high-performance metal-air batteries will benefit from the knowledge obtained from neutron scattering and sophisticated advanced structural modelling.

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Detecting excitonic magnons in $MnPS_3$, using optical methods

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$MnPS_3$ is a layered antiferromagnetic crystal whose coupled optical and magnetic properties make it a promising material for investigating exciton–magnon interactions and magnetoelectric phenomena. I developed a cryogenic optical spectroscopy platform designed to detect exciton–magnon features in the high-energy spectral region and to study their response to externally applied fields.

The experimental system combines a custom optical cryostats with high-resolution spectroscopic instrumentation. Two complementary photoluminescence configurations and a transmission spectroscopy setup were constructed. Transmission measurements are used to characterize the relevant optical and magnon-assisted spectral features and to verify their presence in the investigated $MnPS_3$ samples. Photoluminescence spectroscopy is then employed to optically excite the excitonic transition and detect the weak magnon-assisted sideband accompanying the primary excitonic emission. The two photoluminescence configurations provide complementary excitation and collection capabilities, enabling the measurement of weak spectral signatures under cryogenic conditions.

The platform is also designed to investigate changes in the excitonic and magnon-assisted transitions under applied electric and magnetic fields. Because of the magnetoelectric property of $MnPS_3$, such field-dependent measurements may reveal modifications in the energy, intensity, or polarization of the exciton–magnon sideband. This system therefore establishes a versatile experimental framework for studying the interplay between excitonic, magnetic, and magnetoelectric degrees of freedom in layered antiferromagnetic materials.

Turquoise Hydrogen by Methane Pyrolysis over Ni-Mo/MgO Catalysts: Impact of Different Synthesis Routes on Structure and Activity

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Methane pyrolysis is a promising, low-emission route for hydrogen production, in which methane decomposes into hydrogen and solid carbon ($CH_4 \rightleftharpoons C + 2H_2$) at elevated temperatures [1]. To lower the required reaction temperatures, transition metal catalysts supported on metal oxides have been widely investigated. In this study, an equimolar Ni–Mo/MgO catalytic system (1.2 mmol g^{-1} metal loading) was examined to evaluate the influence of two synthesis methods—wet impregnation (WI) and sol–gel (SG)—on alloy phase formation and catalytic performance. Following synthesis, the catalysts were calcined in air at 550 °C and reduced in H_2 at 800 °C. Isothermal methane pyrolysis was conducted for 3 h in a horizontal quartz tube reactor using a 50% CH_4/Ar mixture under different pre-treatment conditions. Gas products were analyzed by QMS and GC, and the catalysts were characterized using H2-TPR, XRD (with Rietveld refinement), TEM coupled with STEM-EDS, and XPS.

H2-TPR showed complete reduction of the SG catalyst, whereas the WI catalyst reached only approximately 65% reduction. TEM imaging revealed smaller metal particles for WI (5.0±1.5 nm) and larger ones for SG (11.4±2.9 nm). The sol–gel method promoted better co-assembly of Ni and Mo on the forming MgO, resulting in a more uniform distribution of mixed oxides (e.g., NiMoO4) after calcination. Consequently, the reduced SG catalyst maintained a surface Mo/Ni ratio close to 1 (as detected by XPS). At the same time, WI showed ~2.0, indicating partial metal segregation on the pre-formed MgO support (probably Ni-rich alloy species within the pores, and Mo on the external surfaces). XRD confirmed FCC Ni(Mo) and BCC Mo(Ni) alloy phases after reduction, with SG containing about twice the fraction of active FCC Ni(Mo) compared to WI.

The SG catalyst outperformed the WI catalyst, exhibiting higher methane conversion, a lower deactivation rate, and higher yields of hydrogen and carbon nanotubes (CNTs)—particularly after reduction followed by pre-carburization at 550 °C. Increasing the reaction temperature enhanced initial conversion but accelerated

deactivation in both catalysts. Unreduced catalysts showed higher initial activity after an induction period, but they deactivated faster and formed thinner nanotubes. Post-pyrolysis XRD indicated Mo depletion in both alloy phases, accompanied by Mo_2C formation. The superior performance of the SG catalyst is attributed to its complete reducibility and a higher fraction of active, larger-sized FCC Ni(Mo), which provides more active sites for balanced methane dissociation and CNT formation. Future studies will utilize neutron-based techniques, such as PGAA and MTEST, to determine catalyst composition and nanocrystalline phases, thereby complementing existing surface characterization data.

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Brewing Better Materials: Valorization of Spent Coffee Grounds into Carbon-Based Nanomaterials

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Annually, 181 billion tons of organic waste are accumulated globally [1], with the majority dumped in landfills, causing soil contamination and contributing to water pollution. Nevertheless, biomass represents a unique source of renewable organic materials, especially since carbon-based nanomaterials can serve as precursors for obtaining functional hybrid materials and nanoplatforms in many useful applications and help to obtain environmentally friendly chemicals. A vast amount of the aforementioned waste is composed of bio-based industrial and municipal waste, one of the types of which is spent coffee grounds (SCG). The purpose of the current work is to produce valuable carbon nanomaterials from SCGs by means of their thermochemical conversion.

The transformation of SCG biomass into high-value carbon nanomaterials occurred in a series of steps combining slow pyrolysis, standard chemical activation, and microwave-assisted chemical activation approaches [1]. Thus, the biomass was subjected to heat treatment with a heating rate of 5°C/minute and 2 hours isothermal at 600°C. The final activated carbon nanomaterial was obtained by chemical activation (modified Hummer method) and microwave irradiation techniques using the SynthWAVE MA167 microwave system (Milestone, Sorisole, Italy). The materials were purified by neutralization and washing with water, filtration, centrifugation, and dialysis methods.

Preliminary results show that the synthesis conditions affect the morphology and physicochemical characteristics of the obtained biochar and final materials [1]. The materials were further tested for practical application in detection of different analytes from water. The described approach proves the potential applicability of the circular economy model, as agricultural waste can easily become an organic building block of advanced carbon-based nanomaterials.

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Silica-based adsorbents for precious metals and REEs recovery from wastewater

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Precious metals (PM) and rare earth elements (REE) are of great economic importance, being key components in almost all industrial and technological products. The growing demand for PM and REE and their uneven geographic distribution increase supply risk. Moreover, mining and processing of these elements, and discharge of PM/REE-containing wastewater pollute the environment. These supply and environmental risks can be tackled by PM/REE recovery from wastewater using silica-based adsorbents, which can effectively adsorb PM/REE due to their high specific surface area, porous structure, and diverse surface functional groups. Various techniques and methods can be used to elucidate the adsorbent's structure–performance relationships that underpin their PM/REE adsorption efficiency and selectivity. The aim of participating in the CETS is structural characterization of novel silica-based adsorbents using neutron and X-ray based techniques such as SANS and SAXS.

The effect of different salt solution concentrations on bentonite swelling

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In the deep geological repository for high-level radioactive waste, the highly compacted bentonite buffer layer will be subjected to long-term chemical cycling actions from saline groundwater, and the evolution of its swelling performance is critical for the long-term safety assessment of the repository. Existing studies have primarily focused on the swelling inhibition effect during salinization, while the irreversibility of swelling behavior and its underlying micro-mechanisms under salinization-desalinization cycling paths remain insufficiently understood. In this study, Gaomiaozi (GMZ) Na-bentonite was employed to design salinization (0.001→2 mol/L) and desalinization (2 mol/L diluted back to original concentrations) paths of NaCl solution. The evolution of the correlation between the microstructure and macroscopic swelling behavior of bentonite under cyclic chemical actions was systematically investigated through SAXS nano-structural characterization. Preliminary experiments revealed that the desalinization curve is consistently higher than the salinization curve, indicating a significant swelling hysteresis effect; the diluted samples exhibited SAXS bimodal distribution at a concentration as low as 0.06 mol/L, which is attributed to the "ultra-pure Na-saturation" state formed by the irreversible replacement of interlayer Ca^{2+} by Na^{+} during the high-salinity stage. This study elucidates the chemical cycling path-dependent irreversible swelling mechanism, providing a theoretical basis for the long-term performance assessment of buffer materials in the repository.

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