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01

Engineering MOF Thin Films: Linking Architecture, Dynamics and Function

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Metal-organic frameworks (MOFs) are porous materials that can reversibly change their structure in response to external stimuli, making them promising for sensing and separation technologies. Understanding and ultimately controlling these responses requires precise control of thin-film architecture and the ability to follow structural and chemical changes as they occur. Within a two-year postdoctoral CERIC project supporting researchers from Ukraine affected by the war, the corresponding author developed a highly reproducible, semi-automated spin-assisted layer-by-layer liquid-phase epitaxy (LbL-LPE) approach for mixed-linker MOF thin films.a By varying synthesis conditions, the method enables precise control over key structural parameters, including crystallite orientation and size. CERIC's complementary research infrastructure has been central to linking these controlled architectures with their dynamic behaviour. At the SAXS Beamline, synchrotron grazing incident wide angle X-ray scattering (GIWAXS) quantitatively confirms highly oriented films and enables structural transformations to be followed under external stimuli. At the SISSI beamline, grazing-incidence infrared spectromicroscopy (GI-IR) confirms molecular incorporation and probes chemical changes in azobenzene-loaded photoresponsive films. Combining these complementary structural and spectroscopic probes reveals a strong dependence of framework response on crystallite size and orientation, including a critical size below which azobenzene infiltration is suppressed and increasingly pronounced light-induced dynamics in larger crystallites. Crystallite orientation also strongly influences stability, with highly oriented films showing enhanced humidity tolerance compared with defect-rich films and the bulk material. These results provide a foundation for future research linking MOF thin-film architecture with dynamic responses to light and environmentally relevant gases, ultimately establishing design principles for resource-efficient fabrication of MOF thin films with tailored properties for advanced sensing applications.

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02

High-Temperature High-Pressure Cell for In Situ GISWAXS in Hydrogen

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The investigation of structural transformations and degradation processes in materials exposed to hydrogen requires experimental environments capable of reproducing demanding temperature and pressure conditions while maintaining compatibility with synchrotron scattering geometries. Within the ACTNXT project, a compact high-temperature, high-pressure cell is being developed for in situ GISWAXS/SAXS/WAXS experiments at the Austrian SAXS beamline at Elettra.

The cell employs a cold-wall concept combining local resistive heating of the specimen with two independent water-cooling circuits. The design incorporates an Inconel 718 pressure body, single-crystal diamond X-ray windows and a compact reaction chamber intended for operation in hydrogen. The X-ray geometry provides scattering access up to approximately $2\theta = 30°$, with the diamond windows intended for measurements over the 10.4–17 keV photon-energy range. The sample environment is designed for millimetre-sized specimens, typically 3 × 3 mm^2 or Ø4 mm, with a thickness of approximately 0.2–0.5 mm. The current design considers two limiting operating conditions: a high-temperature condition targeting specimen temperatures of approximately 800–850 °C at 50 bar H_2, and a high-pressure condition targeting up to 200 bar at approximately 300 °C.

Numerical thermal and structural analyses were performed to evaluate temperature localisation, cooling efficiency, pressure loading and thermomechanical stresses under the two target operating conditions. The simulations identify the 50 bar/high-temperature regime as the governing thermo-mechanical condition and indicate that the proposed cold-wall architecture can maintain strong temperature localisation while limiting heating of the external pressure body. Current development focuses on the miniature ceramic heater assemblies, optimisation of the critical pressure-boundary geometry, integration with the beamline gas-handling system, and preparation of the design for prototype manufacturing.

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03

Playing with LEGO(like) bricks – building novel virus-like particles

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Virus-like particles (VLPs) are attractive nanocarriers, yet the early stages of icosahedral shell assembly are transient, heterogeneous and poorly characterized structurally. Here we used recombinant coat protein (rCP) of Red clover necrotic mosaic virus (RCNMV) to study in vitro self-assembly with and without cargo (tRNA, RCNMV RNA2, siRNA, and the polyanions PSS and DSS). Mass photometry, DLS and nanoDSF showed that 200 kDa rCP oligomers form before any interaction with RNA, that VLPs larger than 0.8 MDa appear only with cargo, and that cargo raises the melting temperature of rCP by 10-20 °C. To our knowledge, this is the first cryo-EM description of the self-assembly intermediates of an icosahedral virus: cargo-free rCP yields mainly trimers and pentamers of dimers, with decamers of dimers as the largest species (radius ~10.8 nm). Cryo-EM further revealed that the cargo determines VLP architecture. Instead of the native T=3 capsid (180 subunits), rCP formed nonicosahedral particles: D3-symmetric VLPs of 78 subunits with tRNA (2.59 Å), D3 barrel-shaped VLPs of 108 subunits with RNA2 (6.52 Å), D2-symmetric VLPs of 72 subunits with PSS (3.01 Å) and DSS, and a minor D5 form of 90 subunits with DSS. siRNA produced the most heterogeneous population, including D2, D3 (102 subunits) and C2 ring-shaped (56 subunits) particles, all with central cargo density. RNA-filled VLPs displayed layered internal organization, and RNA2 adopted the symmetry of the capsid. Our data suggest that early rCP intermediates can serve as building blocks of these alternative shells.

04

Proteins:G-quadruplex interactions

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G-quadruplexes (G4s) are non-canonical DNA structures formed by guanine-rich sequences and widespread throughout the genome. Their involvement in genome stability and DNA metabolism, together with their association with genetic disorders and cancer, makes understanding their recognition and processing by cellular proteins highly relevant [a]. G4-binding proteins and their complexes with G4s have consequently emerged as potential therapeutic targets. However, the limited selectivity of currently available G4-targeting molecules highlights the need to better understand the molecular determinants governing G4–protein recognition. Here, we investigate the structural basis of G4 recognition by human RecQ helicases, a family of genome-maintenance enzymes that includes RecQ1, BLM, WRN, RecQ4 and RecQ5. Although RecQ helicases are involved in G4 metabolism, their interactions with G4s are not uniform, suggesting that both G4 topology and protein molecular features contribute to recognition [b,c]. A systematic characterization of RecQ helicases with different G4 substrates therefore provides a framework to investigate the determinants underlying binding specificity and interaction modes. We focus also on the N-terminal region of RecQ4, which displays selective affinity for G4 structures [d,e,f]. To dissect the molecular basis of this interaction, we combine biochemical characterization with solution NMR spectroscopy. 1H NMR analysis of G4 imino protons is used to monitor structural perturbations upon protein binding, while 1H15N HSQC titrations provide residue-specific information on the protein side of the interaction. This approach enables us to investigate both G4-dependent effects and the protein regions involved in recognition. By integrating these complementary approaches, this work aims to define how structural features of G4s are translated into selective protein recognition and to provide a molecular framework for understanding G4–helicase interactions. Such knowledge will contribute to a better understanding of G4 metabolism and may support the development of strategies targeting G4-related pathways.

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05

Solid-State NMR Investigation of Lithium Supplementation from Li2C4O4@SiO2 Microcapsules for Extended Cycle Life in Self-Healing Lithium-Ion Batteries

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Microcapsules containing additional lithium salts for lithium-ion batteries (LIBs) are presented here. The microcapsules comprise an outer hollow porous SiO2 shell and an inner core of lithium squarate (Li2C4O4). In LIBs, a long cycle life requires continuous Li+ intercalation and de-intercalation. These processes induce volume changes in electrode materials, leading to continuous reformation of the solid electrolyte interphase (SEI) and consumption of active lithium. Therefore, an additional lithium-ion source is needed to compensate for lithium loss and improve cell lifetime. In this work [1], microcapsules containing Li2C4O4 are investigated as an extra lithium source for the cathode in lithium-metal cells and LIB cells with a graphite-based negative electrode. The microcapsules are air-stable, cost-effective, and compatible with standard industrial electrode processing. The concentration of lithium salt and its effects on electrode and electrochemical properties are studied. Solid-state 7Li MAS NMR is used to investigate the chemical state and mobility of lithium before and after activation. An increase in cycle life of NMC622+Li2C4O4@SiO2||graphite full-cell is reported, which grows linearly with the initial amount of lithium salt due to extra Li+ ions but decrease at higher amount due to parasitic reactions. Although concept of microcapsules is very old term in medical fields but in case of energy storage application it can be revolution.[2,3] Acknowledgements The authors acknowledge funding from the European Union Horizon Europe programme (SALAMANDER, Grant No. 101104028), Horizon 2020 (BATTERY 2030+ CSA3, Grant No. 101104022), and the Slovenian Research and Innovation Agency (ARIS; P2-0423 and P1-0021). The NMR measurements were performed at the Slovenian NMR Centre using equipment provided by

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06

X-ray and Neutron Imaging in Plant Physiology

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With a rapidly growing global population and increasing food demand, securing agricultural productivity and crop resilience is one of the most critical challenges. It requires a deep understanding of how plants optimize nutrient recycling and manage water usage under severe environmental stress. Imaging techniques available at large-scale facilities offer great opportunities to probe these physiological processes across multiple spatial and temporal scales. In the present work, we demonstrate the power of combining X-ray fluorescence and neutron imaging to reveal key physiological adaptation strategies: subcellular metal recycling during leaf senescence and whole-plant rehydration kinetics during desiccation recovery. As neutron radiography is exceptionally sensitive to hydrogen, we have utilized it to track spatial and temporal water movements in the resurrection plant Haberlea rhodopensis during recovery from an air-dry state. By evaluating root vs foliar water uptakes, we visualized distinct pathway efficiencies and spatial distribution patterns governing desiccation recovery. Utilizing the plant model Arabidopsis thaliana, we investigated iron remobilization from chloroplasts during developmental senescence. Lowenergy synchrotron X-ray fluorescence microscopy confirmed localized iron enrichment at chloroplast sites at early senescence stages. However, as senescence progressed, iron level declined. The absence of a characteristic ferritin signal in 57Fe Mössbauer spectra, paired with the stochastic presence of ferritin particles, indicated that chloroplast ferritins act only as dynamic transient compound rather than a permanent storage.

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07

Probing Nanoscale Structure for Long-Term Stability in Organic Solar Cells Using Scattering and Spectroscopy

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Organic solar cells (OSCs) are promising technologies for nextgeneration renewable energy due to their potential for lightweight, flexible, and low-cost photovoltaic applications. Despite significant advances in device efficiency, long-term stability remains an important challenge for their wider deployment. Understanding how changes in the nanoscale structure of the active layer influence device stability is therefore essential for improving their performance over extended operation1.

Here, we investigate the relationship between active-layer morphology, composition, and stability in PTQ10-based OSCs by comparing binary and ternary blend systems2. Although Y6 and Y-Pr share a similar conjugated backbone, differences in their end-group chemistry lead to distinct molecular packing and phase behaviour. AFM and GIWAXS results show that incorporating Y-Pr (20 wt%) reduces domain size and modifies phase separation, resulting in finer nanoscale features. Thermal ageing at 65 °C under inert conditions demonstrates enhanced stability in the ternary system, which retains more than 80% of its initial performance after 1080 hours. To investigate the structural and chemical origins of this stability, we combine synchrotron- and laboratory-based GIWAXS, AFM, infrared and Raman spectroscopy with device performance measurements. Through this research, we aim to identify structural factors governing the long-term stability of OSCs and contribute to strategies for improving their operational lifetime.

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08

Electrochemical Impedance Spectroscopy Analysis of Anion Exchange Membrane Water Electrolyzer

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Anion exchange membrane water electrolyzers are emerging technologies for producing green hydrogen using electricity from renewable sources. They combine the high efficiency and production rates of proton exchange membrane electrolyzers with the use of non-noble-metal catalysts characteristic of alkaline electrolyzers. To optimize catalyst layers and improve electrolyzer performance, it is essential to obtain detailed information from operating devices. Electrochemical impedance spectroscopy, combined with the distribution of relaxation times, enables the separation of individual contributions to overall electrolyzer losses, including those associated with the hydrogen and oxygen evolution reactions. This approach enables the characterization of individual components and supports targeted optimization. To facilitate the analysis of the large volume of impedance data collected at our testing stations, we developed eisyFIT, a Python-based software tool employing machine-learning algorithms.

09

Unlocking stimuli-driven dynamics: A multi-technique approach to characterize responsive systems

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Responsive crystalline materials that undergo controlled structural transformations upon external stimuli offer exciting opportunities for applications such as gas capture, sensing, and molecular separation. A key challenge, particularly for thin-film systems, is to accurately characterize their structural dynamics and establish their relationship with functional performance. Using flexible metal-organic framework (MOF) films as a model system, we investigate the interplay between framework structure, morphology, chemical environment, and gas uptake under low-pressure conditions. $Zn_2(BDC)_2DABCO$, featuring dinuclear zinc-carboxylate units, serves as a model system to investigate the reversible structural response associated with CO_2 adsorption and desorption. To resolve these interdependencies, we employ a complementary multi-technique approach combining grazing-incidence X-ray scattering, infrared spectromicroscopy, quartz-crystal microbalance (QCM) measurements, and morphological and surface-sensitive characterization. The combination of structural and spectroscopic techniques enables us to correlate framework orientation and structural changes with local chemical environments, while QCM measurements provide quantitative insight into mass changes during gas uptake and release. Beyond conventional film fabrication, we demonstrate the applicability of the approach to layer-by-layer liquid-phase epitaxy (LbL-LPE), enabling the controlled preparation of highly oriented MOF thin films and facilitating the investigation of their responsive behaviour. Our results demonstrate how combining complementary characterization techniques with controlled thin-film fabrication strategies can unravel dynamic structure–property relationships in responsive MOF systems. This approach provides a foundation for understanding and tuning switchable gas uptake and reversible low-pressure CO_2 capture in flexible crystalline thin films.

10

Recognition and structurization of DNA G-quadruplex aptamer by RG-rich peptides

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Interactions between proteins and nucleic acids are crucial for the regulation of many cellular pathways. However, exact mechanisms at the atomic level are often still poorly understood due to difficulties in vitro mimicking of intracellular conditions that are needed for breakthrough structural studies. One example of such important biological interactions are the ones between non-canonical nucleic acid secondary structures called G-quadruplexes and the arginine/glycine-rich (RGG/RG) domains of DNA/RNA binding proteins.1 G-quadruplexes are structurally diverse and capable of performing a broad range of cellular functions, most notably regulation of gene expression, which may be facilitated by the binding of various DNA or RNA processing proteins. Nucleolin, a multifunctional nucleolar protein, contains an intrinsically disordered C-terminal RG/RGG-rich domain. It plays a role in various cellular functions and is also capable of G-quadruplex binding.2

We investigated the interaction between the nucleolin-derived RG/RGG-rich peptides and an antiparallel TBA G-quadruplex, a well-established DNA G-quadruplex model. We show that the investigated binding has moderate strength and that the binding is influenced even by the smallest differences in the amino acid sequence of RG/RGG-peptides, while a specific amino acid sequence may be responsible for the major contribution towards the binding affinity. Binding strength and stabilization of G4 structures is heavily impacted by arginine sidechain methylation, a well-known post translational modification. Interestingly, we show that TBA oligonucleotide adopts a G4 topology in the presence of RG-rich peptide even in the absence of the G4 promoting cations. Our high-resolution structural results of the interaction may become of greater interest considering the importance of the investigated interaction for the development of G-quadruplex-based anti-cancer aptamers that are incorporated into the target cells via interaction with nucleolin protein.

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11

Developping Fe3O4@CeO2 magnetic nanocomposites for treating systemic disorders and skin lesions

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Radiation injury to humans is not limited to situations of military confrontation, but can also occur in peacetime. Radiation-induced health damage in patients undergoing radiotherapy leads to systemic and skin problems manifested as burns; accidental radiation exposure of personnel in special facilities and laboratories working with or exposed to radioactive sources occur despite widespread education, training and the highest quality safety measures. The known effects of excess radiation can be classified as thermal. They are similar to those of electrical burns with some unique systemic manifestations.

Preliminary obtained data showed successful pilot fabrication of the magnetic Fe3O4@CeO2 nanocomposites, which possess a significantly higher antioxidant activity in comparison to both individual components due to the socalled "chemistry-based" synergetic effect. These preliminary data suggest that a significant therapeutic effect can be expected from the combined use two varieties of nanocomposite-based multi-component hydrogels for internal therapy aimed at eliminating systemic disorders (in particularly, oxidative stressrelated damages) caused by acute radiation sickness and for the external therapy of radiation-induced wounds and burns. However, the nature of this effect remains an open scientific question and should be studied in more detail.

For this study, new magnetic Fe3O4@CeO2 nanocomposites were synthetized in order to optimize antioxidant and radioprotective properties. The nanocomposites were investigated using Transmission Electron Microscopy techniques (CTEM, SAED, HRTEM, EDS and EELS). CTEM was used to determine the morphology of the nanoparticles and the size distribution. HRTEM and SAED were used to identify the crystalline structure. EELS-SI was used to determine the distribution of cerium oxide nanoparticles relative to iron oxide nanoparticles.

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UV and Deep X-ray Litography for interisciplinary research

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The combination of top-down processing through micro/nano fabrication techniques with bottom-up approaches to prepare novel functional materials finds increasing interest, as it has great potential to achieve next generation of lab on chips, of portable microsensors, of energy harvesting and catalysis systems. Bottom-up methods rely on chemical reactions and molecular self-assembly, where the material is organized through molecular interactions and chemical equilibria during deposition processes. Exposure to a radiation source can lead to modifications of the materials properties, enabling their patterning. Moreover, irradiation can promote the in-loco synthesis of novel materials. As top down processes we selected both UV lithography and Deep X-ray lithography (DXRL). The latter is based on controlled irradiation of materials using high energy X-rays, and it is advantageous with respect to resolution, penetration depth, high aspect ratio, and vertical sidewalls. Both techniques have traditionally been employed to fabricate components like microfluidics, micro-optics, micromechanics and microelectronics. More recently, DXRL has been exploited in the irradiation of novel materials and in the study of the related structural and functional changes In the poster we will report examples of the latest research on UV and X-ray irradiation at the DXRL beamline and microfabrication laboratory of Elettra synchrotron, which are accessible instruments of CERIC-ERIC through the austrian partner facility. We will describe the patterning of Metal Organic Frameworks (MOFs) to obtain a methanol vapor sensor (a), and of 3D oriented MOFs and MOF templated polymeric films to get microstructures with anisotropic fluorescent properties (b). Then we will describe a microfluidic device which is transparent to UV-visible light in one direction and to X-rays in the perpendicular one, to study of photoactive systems using visible spectroscopy and/or Small Angle X-ray Scattering (c).

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Probing the Electrochemical Dealloying Behaviour of Platinum-Based Bimetallic Oxygen Reduction Reaction Catalysts

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Bimetallic Pt-based alloy catalysts are attractive alternatives to pure Pt for the oxygen reduction reaction, but their long-term durability remains a central obstacle to practical deployment. Understanding when and how alloying elements are lost during operation is therefore essential for rational catalyst design. We investigate model Pt3M (M = Cu, Ni, Co) thin-film catalysts, prepared by magnetron co-sputtering with matched stoichiometry, thickness and morphology, combining accelerated degradation testing (ADT) with time- and potential-resolved scanning flow cell ICP-MS (SFC-ICP-MS). This approach isolates the effect of alloying-element identity from structural and morphological variables, and links electrochemical activation and degradation directly to elemental dissolution. ADT shows that Pt3Co and Pt3Ni activate rapidly but degrade most severely, while Pt3Cu activates slowly yet retains the smallest surface-area loss over extended cycling. Time-resolved SFC-ICP-MS traces this divergence to the very first seconds of electrolyte contact. Pt3Co and Pt3Ni lose a substantial fraction of their Co and Ni loading immediately upon contact, while Cu dissolution from Pt3Cu is initially negligible. Over subsequent cycling, however, Cu dissolution accelerates and ultimately exceeds the cumulative alloying-element loss of Pt3Co and Pt3Ni. Long-term stability is thus governed not only by how much alloying element is lost, but by when that loss occurs, establishing initial electrolyte exposure as a decisive stage in Pt-alloy catalyst evolution.

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Insight into the morphological and structural properties of nanostructured NiO with applications in CO sensing

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Nickel oxide (NiO) is a p-type semiconductor which exhibits remarkable electronic, catalytic and structural properties. Moreover, its chemical stability makes this material suitable as a sensing layer for chemoresistive gas sensors [a]. The present study is focused on characterizing the morphological and structural properties of NiO nanoparticles synthesized by hydrothermal route and calcined at 400 °C and 500 °C. The structural properties of the two samples were determined using X-ray Diffraction (XRD), while the morphology and microstructural properties were identified by using different transmission electron microscopy (TEM) techniques: Conventional TEM (CTEM), Selected Area Electron Diffraction (SAED), High-resolution TEM (HRTEM) and Scanning TEM combined with Energy Dispersive X-ray Spectroscopy (STEM-EDS). XRD, SAED and CTEM results showed that the sample calcined at 500 °C has larger nanoparticles and a higher degree of crystallization compared to the one calcined at 400 °C. Moreover, HRTEM imaging provided valuable insights into identifying the growth mechanism of the larger nanoparticles calcined at 500 °C [b]. Considering the morpho-structural characteristics of these two materials, the sensor signal was expected to be larger for the sample calcined at 400 °C, but our results showed the contrary. To understand this atypical result, we performed an in-depth study at atomic scale using Electron Paramagnetic Resonance Spectroscopy (EPR), SAED and STEM-EDS and the results revealed the presence of metallic nickel clusters at the surface of NiO nanoparticles in both samples. These clusters influence the electrical conductivity of NiO, thus justifying the peculiar sensor signal [c].

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SOLARIS: Research Infrastructure and Capabilities — Applications in Cultural and Natural Heritage Research

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The SOLARIS National Synchrotron Radiation Centre in Kraków is the only synchrotron light source in Central and Eastern Europe. Since opening to users in 2018, the facility has been providing access to advanced research infrastructure based on synchrotron radiation, including beamlines operating in the infrared, ultraviolet and X-ray ranges, as well as complementary instrumentation such as cryo-electron microscopy. SOLARIS enables the application of a broad range of analytical techniques for structural, chemical and morphological characterization across multiple length scales. The available experimental methods support research in materials science, physics, chemistry, life sciences, environmental studies and heritage science, including investigations of unique and irreplaceable samples for which non-destructive or minimally invasive approaches are required. This contribution presents the current research infrastructure available at SOLARIS together with ongoing developments of the facility. Particular attention will be given to opportunities for cultural and natural heritage research. Synchrotron-based techniques available at SOLARIS have been successfully applied to the study of archaeological materials, fossil remains and ancient biological systems, providing information on chemical composition, molecular structure, preservation processes and three-dimensional morphology. These examples demonstrate how complementary use of infrared spectroscopy, X-ray spectromicroscopy and X-ray imaging methods can support the characterization of heritage objects and contribute to a better understanding of their origin, history and state of preservation. Overall, the presentation will highlight the capabilities of the SOLARIS infrastructure and its potential to support interdisciplinary research involving heritage materials, from the microscale to the nanoscale.

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Unveiling the Structural Landscape of pSNCA-G4: A Four-Quartet Antiparallel G-Quadruplex as a DNA-Level Target for Parkinson's Disease

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Alpha-synuclein (α-Syn), encoded by the SNCA gene, is a key protein implicated in synucleinopathies, including Parkinson's disease[1]. We recently identified a distinct regulatory target at the DNA level: a G-quadruplex (G4) located at the SNCA transcription start site (pSNCA-G4)[2]. Biophysical and cellular studies demonstrated that pSNCA-G4 is a stable and functional regulatory element. Notably, an antisense peptide nucleic acid conjugate designed to selectively disrupt pSNCA-G4 reduced both SNCA mRNA and α-Syn protein levels by over 70% within 24 h. This pronounced and rapid effect, exceeding the 25–50% reduction generally considered pharmacologically meaningful, establishes pSNCA-G4 as a compelling target for α-Syn modulation. To enable selective small-molecule recognition of this target, we performed an extensive NMR investigation of pSNCA and related extended and mutant sequences. The data revealed a highly polymorphic conformational landscape comprising multiple G4 species, identifying a predominant antiparallel architecture containing four G-quartets. Mutational analysis indicated that the G4 core is largely conserved, whereas structural polymorphism mainly arises from differences in loop composition and strand progression. pSNCAext2 displayed two major structural species, the populations of which were influenced by the length and composition of the second and third loops. NOESY correlations supported an antiparallel topology with four G-quartets and eight syn-anti steps. Together, these findings establish pSNCA-G4 as a pharmacologically relevant regulatory target for α-Syn expression and provide a structural framework for exploiting its conformational plasticity. Loop-dependent structural differences, together with the four-G-quartet antiparallel architecture and groove features, provide a rational basis for designing hyperselective ligands able to recognize a specific pSNCA-G4 topology, opening a new avenue for chemical modulation of SNCA expression directly at the DNA level.

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Clustering-Based Quantitative Nanoparticle Characterization Using Scanning Electron Diffraction

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Scanning electron diffraction provides spatially resolved crystallographic information but its analysis becomes challenging when several nanoparticles overlap in projection and contribute simultaneously to the recorded diffraction pattern. Conventional automated orientation-mapping approaches generally rely on matching each local pattern to simulated templates and assigning a best phase or orientation, while recent clustering-based methods have shown that recurring diffraction features can instead be used to separate overlapping structural contributions [a,b]. Here, a clustering-based workflow was applied to BaFe12O19 nanoparticle [c] assemblies with frequent particle contact and overlap. Selected regions of diffraction space were used to generate virtual images whose combined intensity information was grouped into representative components and subsequently reconstructed under non-negative constraints. This allowed multiple contributions to coexist at the same scan position rather than forcing an exclusive assignment to a single particle. The resulting spatial component maps enabled individual particle regions to be recovered and quantitatively analyzed. Their projected shapes were characterized by ellipse fitting, allowing an automated particle-size distribution to be obtained. The distribution was consistent with independent manual TEM measurements. The approach therefore provides a robust route from scanning diffraction data to quantitative nanoparticle morphology, particularly for crowded assemblies where conventional image-based segmentation or singlepattern indexing can become ambiguous.

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Combing iSCAT and biological sentinels for the rapid detection of airborne viral particles

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The COVID-19 pandemic and the recent public health alarm over viruses such as Hantavirus and Ebola have underscored the critical need for rapid technologies to detect airborne pathogens directly in environmental air samples. To address this challenge, we employed an interferometric scattering microscope (iSCAT), a recent powerful label-free method, capable of achieving single-particle sensitivity. To build a predictive framework, we initially implemented Mie scattering simulations using the T-Matrix formalism, coupled with geometric parameters derived from electron microscopy (EM). This computational approach enables precise modelling of non-spherical and multi-layered particles, effectively accounting for the core-shell structures typical of enveloped viruses, distinguishing them from common environmental aerosols (e.g., black carbon, brown carbon, nanoplastics). Combining these simulations with multispectral profiling allowed the identification of distinct spectral signatures that differentiate viral particles from background particulate matter. Experimentally, we then spectrally characterized a set of reference nanoparticles (polystyrene, silica, and polyvinyl chloride), together with viral particles. The resulting datasets were used to train a Machine Learning algorithm for the automated identification of pathogens directly from experimental z-stacked interferograms. In parallel, biological selectivity can be achieved by using DNA aptamers, tailored to selectively bind and immobilize target viral families. The specificity and binding affinity of these aptamers toward their respective viral targets were rigorously evaluated and validated via Surface Plasmon Resonance (SPR), ensuring high-performance biorecognition.

These synthetic receptors allow for the high-affinity capture of pathogens from complex matrices, while the iSCAT detection provides real-time, multidimensional analysis of the individual immobilized particles.