Book of Abstracts

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Contents

Speakers' abstracts

Beyond the Bench: Career Transitions into Scientific and Public Leadership

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Thursday afternoon, November 14th

How do we navigate the landscape of truly interdisciplinary research? How can a core scientific concept be approached from multiple vantage points to generate nationally significant projects? And how does one transition from a laboratory-based faculty role to positions such as Deputy Scientific Director at CNRS or Research Advisor in a ministerial cabinet?
These are the questions I'll address in this talk, drawing on concrete examples and lessons learned along the way.

Material and polymer chemistry for the preservation of cultural heritage

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Friday morning, November 14th

Heritage science, at the intersection of the humanities and natural sciences, uses engineering and materials physical chemistry to address key challenges: understanding, preserving, and restoring cultural objects. This presentation will illustrate this connection through three research projects I co-led in the field of conservation-restoration:

- Strengthening heritage papers with a polymer-based treatment for simultaneous deacidification and consolidation;
- Investigating the dyeing properties of wild silks to explain their reactivity differences;
- Developing compatible plasters for earthen constructions by incorporating bio-based polymers to enhance their durability.

This work shows how physical-chemical analyses reveal the composition and properties of cultural heritage materials, and how innovative, often polymer-based treatments can stabilize fragile objects and improve their durability. We will also address the need to adapt these practices to contemporary environmental challenges by developing sustainable solutions in conservation-restoration.

Industrial decarbonisation

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Friday afternoon, November 14th

The French industrial sector accounts for approximately 18% of national greenhouse gas (GHG) emissions. Industrial decarbonization will necessarily rely on energy efficiency measures and the substitution of fossil fuels with renewable energy sources. However, these levers alone will not be sufficient, as several long-established industrial processes are inherently carbon-intensive. This is notably the case for the production of aluminum, ammonia, steel, and cement. Alternative solutions are emerging but remain slow to deploy and require substantial industrial research efforts. Strengthening interfaces between research institutions and industry is therefore more critical than ever to accelerate the energy transition and ensure compliance with our climate commitments.

Thursday, November 13th

Operando Sensing For Green Hydrogen Production

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Poster 7

Keywords: Alkaline Electrolyzer ; Green Hydrogen ; Optical Sensors ; Tilted Fiber Bragg Grating

Monitoring Alkaline Electrolyzer Health Through Optical Sensors

Water alkaline electrolyzers represent a promising technology for the long-term energy transition as they have the advantage to produce carbon-free hydrogen when using renewable energy. However, despite extensive industrial development, sustainability challenges persist due to fast electrolyte degradation induced by component corrosion. In this study, we propose an innovative approach by incorporating optical tilted fiber Bragg grating (TFBG) sensors into an alkaline electrolyzer to monitor operando electrolyte composition and corrosion by-products. We show that by tracking variations of turbidity in the electrolyte, we can assess the concentration of suspended iron oxide and hydroxide particles. Simultaneously, TFBG sensors can allow us to follow temperature changes coming from pore blockage of the membrane. Our study presents an innovative solution to monitor operando the electrolyte of alkaline electrolyzers, helpful for electrolyte thresholds and electrode degradation.

Heterogeneous acids for visible photo-driven oxidative upcycling of polystyrene

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Poster 19

Keywords:

Polystyrene (PS) is used in many everyday objects and in laboratories (yoghurt pots, spectrophotometry cells, etc.). About 17 million tonnes of PS are produced worldwide each year1. PS is fairly stable and can become a pollutant if not properly managed after use. The current trend is to consider chemical recycling, either to return to styrene (pyrolysis) or to produce valuable molecules (upcycling) such as benzoic acid by the oxidative cleavage of carbon chains2. In this work, we focused on the development of a photocatalysis approach that i) avoids unstable photosensitizers and ii) favours heterogeneous catalysts which are active under visible light irradiation. Our starting point is the described activation of PS aromatic rings by protons, enabling PS to be responsive to visible light, thereby activating oxygen to 1O2, which is involved in the oxidative cleavage of PS under O2. Herein, Nafion® resin (proton density: ∼0.9 mmol/g) was chosen as the heterogeneous acid catalyst due to its chemical resistance and super-acidity. Under illumination with Blue LEDs, PS with Mn of c.a. 180,000 g/mol was converted into benzoic acid (BA) with 71% yield in 40 h and residual PS oxide of very low molecular weight (Mw: ∼500). Nafion® could be recycled four times (total time: 200 h) although it was slightly degraded according to XPS, FT-IR and the decrease of proton density. Furthermore, this catalytic system also showed promising results (BA yield from 43 to 70%) for the degradation of PS from many everyday objects, i.e. involving additives. Concerning the mechanism, PS would be activated by heterogeneous acids and excited upon irradiation in the visible range, thereby producing 1O2 from 3O2. Then, PS would be oxidized to PS oxide, BA, and formic acid. Due to the effects of protons, PS oxide, and π-π interactions, the BA yield reaches up to 71%.

Atomic-Scale Insights into the Hydration of Low-Index Rb2Ti2O5 Surfaces

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Poster 9

Keywords: ionic conductor ; density functional theory ; perovskite ; proton conductor ; modelisation ; oxyde titanate ; oxyde ; interface ; surface ; hydration

The layered oxide Rb2Ti2O5 has recently emerged as a promising solid electrolyte, exhibiting remarkable ionic conductivity and dielectric properties at room temperature under humid conditions. While these macroscopic features are influenced by water incorporation, the atomic-scale behavior of its surfaces—crucial for understanding interfacial reactivity and ion transport—remains largely unexplored. Using density functional theory (DFT), we investigate the atomic structure, thermodynamic stability, and water reactivity of the three low-index surfaces, (100), (010), and (001), of Rb2Ti2O5 [benas], considering only stoichiometric, unreconstructed terminations. Among these, the (001) surface is the most stable, with a surface energy significantly lower than typical oxides. The minimal changes in atomic and electronic structure highlight the quasi-two-dimensional nature of Rb2Ti2O5.

Water adsorbs spontaneously in molecular form, forming ordered layers bound by short hydrogen bonds, with minor disruption to the surface. At higher hydration levels, the (001) surface reaches near-zero surface energy, suggesting spontaneous exfoliation into hydrated sheets. Pronounced outward relaxation of rubidium upon hydration may promote alkali cation solvation, consistent with experimental observations. Hydration relaxes surface stress and stabilizes terminations, yielding thermodynamically stable states even at low water partial pressures. The (100) surface is highly reactive, forming a hydroxylated termination with significant adsorption enthalpy. The hydrated (010) surface supports multiple metastable configurations, with possible hydroxylation via low-barrier water dissociation.

These findings reveal water's dual role: stabilizing surfaces and, through its interaction with the material, potentially initiating bulk proton incorporation and the formation of additional chemical species. This work provides a foundation for future studies of hydration-driven phenomena, surface dynamics, ion transport, and machine-learned simulations.

Simulations of electrochemical systems with flexible electrode models

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Poster 77

Keywords: carbon nanoporous electrochemistry MD MLIP

Electrochemical energy storage devices, such as batteries and supercapacitors, play an important role in the ongoing energy transition. To further optimize their performance, a deep understanding of these devices is crucial. Atomistic simulations provide a unique opportunity to model these systems at the atomic scale under various operating conditions. Recent advancements have enabled explicit modeling of processes like supercapacitor charging.

However, current approaches often simplify electrode models, neglecting their mechanical dynamics, which may impact results, especially when coupled with ion dynamics. It seems interesting to integrate Machine Learning Potentials, which are particularly effective for short-range interactions, with long-range physical models for describing electrostatic interactions. Testing the influence of the electrodes dynamics with several potentials such as AIREBO or the Atomic Cluster Expansion potential demonstrated promising results, revealing discrepancies in key supercapacitor properties across models used for electrode dynamics.

Recent simulations showcased a notable decrease in charging time and increase in capacitance for flexible electrodes models, motivating further exploration into the influence of electrode dynamics on supercapacitor performance. Drawing inspiration from studies on carbon electrode morphology, our study is focused on a system composed of graphitic nanoporous electrodes in contact with ionic liquid electrolyte. Using recent advancements in the Performant Atomic Cluster Expansion model, the objective of this work is to understand the relationship between electrode dynamics, capacitance, and ion adsorption mechanisms. This research not only advances fundamental understanding but also holds promise for optimizing future energy storage device design and performance.

Development of vitrimer-based composites as photovoltaic modules front sheets

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Poster 67

Keywords: Composite ; vitrimer ; photovoltaic ; solar ; epoxy

Photovoltaic (PV) modules typically incorporates an encapsulant made of an adhesive thermoset elastomer and a glass front panel. Replacing glass with composites is an important weight saving opportunity for wider implementation on existing structures. However, no efficient recycling process, allowing to easily sort the different materials of interest, exists for such modules. In this work, we propose to use vitrimer chemistry to create a depolymerizable front sheet.

We sought to adapt typical vitrimer formulation to insure transparency, low cure yellowing, mechanical properties typical of PV polymer front sheets and compatibility with composite manufacturing used for photovoltaic modules. To address these goals, precursors were carefully chosen: epoxy resins, crystalline acid hardeners and organic or metal catalysts.

However, these formulations showed precipitation of insoluble metal carboxylates, impairing vitrimer properties. We tackled this problem with a simple and upscalable synthetic method, giving important insights on catalysis in vitrimer systems. We applied this strategy to our formulation and met required mechanical properties, showed transparency comparable to typical photovoltaic grade polymer matrixes and demonstrated the complete depolymerization of the network activated by the catalyst.

MOF-based composites as Li-ion solid-like conductors

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Poster 79

Keywords: Porous Materials ; Metal ; Organic Frameworks ; Solid ; State Batteries

Metal-Organic Frameworks (MOFs) have emerged as good candidates for energy applications in the quest for new ionic conductors. MOFs are porous materials resulting from the assembly of metal ions/clusters and organic ligands. Their versatile compositions, ordered channels, and tunable porosity offer the required structural features for potential applications in ion batteries. In Li metal batteries, MOF-based ionic conductors can be classified into two types: MOF-incorporated polymer hybrids and liquid electrolyte-laden MOF hybrids. The structure of MOF will affect Li+ diffusion, but the current mechanism remains unclear. Hence, establishing a structure-property link and clarifying the ionic diffusion properties with MOF structures is significant.

In this work, a titanium-based metal-organic framework (Ti-MOF), MIP-207, and its sulfonated analogue, MIP-207–SO_3H, were employed to investigate the influence of –SO_3H and –COOH functional groups on Li^+ percolation behavior. MIP-207 consists of Ti_8O_8 oxo-clusters coordinated with 1,3,5-benzenetricarboxylic acid linkers, whereas partial substitution (16, 28, 44%) with 5-sulfoisophthalic acid leads to the formation of the structurally analogous MIP-207–SO_3H. By introducing LiTFSI in propylene carbonate (PC) into the pores of both MOFs, the ionic conductivity of the resulting composites was evaluated using potentiostatic electrochemical impedance spectroscopy (PEIS) in a solid-state configuration. The ionic conductivity was found to increase with the -SO_3H group content, confirming its role in facilitating Li^+ transport. To further demonstrate the practical potential, MOF-based composite membranes were fabricated and assembled into $Li_{1/2}LiFePO_4$ full cells. The cell employing the MIP-207–SO_3H-containing membrane exhibited superior electrochemical performance compared to the MIP-207-based membrane, highlighting the benefit of sulfonic acid functionalization in promoting Li^+ conduction and interfacial stability.

Towards Novel Nanophotonic Interfaces with Rare-Earth Ion-Doped Nanomaterials

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Poster 3

Keywords:

Rare-earth ions, embedded in crystalline matrices, exhibit remarkable optoelectronic properties: long-lived and coherent optical and spin transitions with narrow, stable spectral lines, spanning a broad spectrum from the ultraviolet to the infrared. To harness these ions as photon or qubit sources, they must be integrated into nanophotonic platforms capable of confining and manipulating light at the nanoscale. For this purpose, materials such as Silicon-on-Insulator (SOI) or III-V semiconductors (GaAs, AlGaAs, GaInP) are preferred. Their fabrication relies on established techniques such as epitaxial growth (MOVPE), electron beam lithography (e-beam), and inductively coupled plasma etching (ICP-RIE). These processes make it possible to structure photonic crystals capable of confining light in cavities or waveguides of dimensions comparable to the wavelength.

The work presented here follow the three steps necessary for the conception of a nouvel light-matter interface: design, fabrication, and characterization. First, the design of photonic cavities using Guided Mode Expansion (GME) simulations and optimization by Inverse Design for Ytterbium's 978 nm optical transition within a GaInP photonic platform. Then, the nanofabrication in cleanroom of such cavities. And finally, the assembly of a confocal microscope setup capable of characterizing both the cavity resonance and the coupled rare earth ion enhanced emission.

Thermo-oxidative ageing of filled elastomers for electrical cable insulation: Correlations between ^{1}H solid-state NMR and mechanical testing

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Poster 8

Keywords: elastomers ; Solid state NMR ; Thermo ; oxydative aging ; network topology ; mechanical properties

The total length of electrical cables amounts to about 1500 km per reactor unit of nuclear power plants. The targeted replacement of the wire insulators is challenging and incurs significant costs, making these components critical. The objective of this study is to assess the possibility to monitor their ageing behavior using and validating a non-destructive technique, solid-state NMR.

This work focuses on the analysis of the thermo-oxidative ageing of EPDM-based model materials filled with aluminum trihydrate (ATH, micrometric), silica (nanometric), ATH and silica and carbon black (nanometric). The presence of ATH particles, used as a filler, has been shown to affect the thermo-oxidation ageing of EPDM rubbers. Nevertheless, the influence of other fillers used in the electrical cable industry on the thermo-oxidative ageing and the synergy between them has been poorly addressed in the literature. The evolution of the network topology under ageing is investigated at the macromolecular scale using solid-state NMR, and the results are correlated with macroscopic mechanical tests (tensile tests) to establish structure–property relationships throughout the aging process. NMR measurements indeed leads to the fraction of elastically active chains, dangling chains, extractibles and also to the distribution of the crosslink density within the EPDM matrix. Such data provide insights into the degradation mechanisms of the EPDM matrix, in particular chain scission and crosslinking phenomena.

An EPDM matrix filled with 30 phr of ATH exhibits an increase in the fraction of elastically active chains with time of thermo-oxidative ageing at 130°C. Such a feature, which suggests

crosslinking of EPDM chains, differs from the behaviour reported in the literature for EPDM networks without any plasticizer. Such a difference suggests that these additives may play a role in the ageing of filled crosslinked EPDM. This study will provide a better understanding of the thermo-oxidative ageing of industrial formulations.

Stabilizing Blue-Phase Liquid Crystals Using Gold Nanoparticles

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Poster 81

Keywords: blue phase liquid crystal ; gold nanoparticles ; SAXS ; liquid crystal

Blue phase liquid crystals (BPLC) are self-organized double twisted cholesteric liquid crystal (CLC) materials exhibiting a Bragg-type selective reflection. Various blue phases (BP) are observed in a small temperature range between the isotropic and the cholesteric phases of CLCs with relatively short pitch [1]. During cooling, three types of BPs are formed depending on the chirality of LC: blue phase III (BP-III), BP-II, and BP-I [2], [3], [4], BP-III is characterized by double twisted cylinders (DTC) with random orientation, while BP-II and BP-I are three-dimensionally ordered simple cubic (SC) and body-centered (BCC) crystals of DTC, respectively. In BP-II and BP-I, discontinuous points exist where the DTCs are in contact, and DTCs and disclination defects coexist [5].

BP have a great technological potential but a main limitation of application by narrow temperature range. Stabilization of the blue phase could be achieved by using molecules with hydrogen bonds [6], mixed with polymers [7] or mixed with nanoparticles (NPs) [8]. Filling disclinations with nanoparticles (NPs) lowers the energy cost, stabilizing the composite and widening its temperature range, though the roles of NP size and surface functionalization in this stabilization remain unclear. NPs also contribute their intrinsic properties, enabling new functionalities in BPLC–NP composites—for example, the plasmonic response of gold NPs.

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In Situ Monitoring of Electron and Ion Conduction in Solid-State Cathode Composites

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Poster 62

Keywords: batteries ; electronic transport ; ionic transport ; coating

All-solid-state batteries (ASSBs) employing Ni-rich layered oxides such as $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) as cathode active materials, paired with sulfide-based solid electrolyte Li_6PS_5Cl, hold great promise as high-energy-density alternatives to conventional Li-ion batteries. However, their performance remains constrained by cathode-related limitations, namely, interfacial reactivity, high tortuosity, and mechanical degradation associated with NMC811 volume changes during cycling—mechanisms that remain poorly understood.

To address these challenges, we investigate transport properties of NMC811:Li_6PS_5Cl composites. Building on recent advances in *in situ* monitoring of electronic conductivity, this work introduces a complementary technique to track the ionic conduction of the cathode composite during cycling. Both electronic and ionic conductivities exhibit an initial increase upon delithiation, attributed to enhanced interparticle contact driven by a cell pressure build-up of approximately 7 MPa, followed by a decline linked to NMC–NMC contact loss at higher states of charge. *In situ* electronic conductivity measurements performed at cycling pressures between 50 and 150 MPa confirm the influence of pressure on electronic percolation pathways, with the conductivity decline becoming more pronounced at 50 MPa.

Furthermore, we examine how the morphology and surface coatings of NMC811 affect electronic transport. Although overall conductivity values remain comparable for single-crystalline (SC) and polycrystalline (PC) NMC811, PC-NMC811 shows lower conductivity at the end of discharge, attributed to secondary particle cracking. $LiNbO_3$ coatings on SC-NMC811 reduce electronic conductivity yet remain stable over 30 cycles. In contrast, $LiNbO_3$-coated PC-NMC811 exhibits higher conductivity than the pristine material. SEM analysis reveals that atomic layer deposition induces partial breakage of secondary particles, altering particle size distribution and enhancing electronic transport.

Altogether, tracking of electron transport in composites provides an approach to probe their mechanical behavior and assess coating durability. When combined with ionic conductivity measurements, these techniques establish a foundation for future studies on solid-state charge transport and diffusion in cathode active materials.

A Chemical Insight in the Chauvet Cave: Analytical Development and Archaeological Interpretation

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Poster 12

Keywords: Rock art ; UV fluorescence ; SWIR spectroscopy ; Heritage studies

The Chauvet Cave (Ardèche, France) is an exceptional Paleolithic site listed as a UNESCO World Heritage Site. With artworks dated at 38,000 years cal BP, it preserves the oldest figurative paintings known to date. For nearly twenty-five years, a multidisciplinary scientific team has been studying the cave, gradually revealing its complexity. However, the physical and chemical study of the site faces a major challenge: the remarkable preservation of the archaeological floor — with visible footprints and objects left on the ground — prevents researchers from approaching the decorated walls closer than a few meters. This working distance makes it impossible to employ the analytical techniques typically used in Cultural Heritage science. To meet this challenge, instruments were developed to perform near-IR reflectance spectroscopy and UV fluorescence spectroscopy non-invasively inside the cave. The analytical approach based on these two complementary techniques enabled to study the stratigraphy of the decorated wall including the limestone substrate, the pigment, and the calcium carbonate concretions covering it. Indeed, UV fluorescence revealed the natural growth of calcite on the works. Characterizing these natural "varnishes" is crucial to understanding the conservation of paintings. As for the near-IR spectroscopy, it has proved to be a rich source of information on the charcoals used as pigments. In parallel with the measurements taken in the cave, analogous materials were synthesized and characterized in the laboratory to reproduce both the pigments used at the time and the evolution of materials over nearly 40,000 years. This approach resulted in a deeper characterization of the technical choices made by Paleolithic artists.

Advanced Characterization of the Chemical Structure of Chitosans Using Capillary Electrophoresis

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Poster 64

Keywords:

Chitosan is one of the polysaccharides that are mostly found in living organisms and second most abundant natural polymer. Owing to the biocompatible, bioresorbable, bacteriostatic and non-toxic properties, chitosan became a promising polymer as cosmetic ingredient, food packaging, biomedical materials and so on. The degree of acetylation (DA) of chitosans is an important parameter that influences their various properties including biological, physicochemical and mechanical properties.

We showed that capillary electrophoresis (CE) can separate chitosans by their chemical composition. Herein, the weight average DA values of chitosans were calculated from the composition distributions. More importantly, this allows the first quantification of their heterogeneity in terms of molecular structure using dispersity but also standard deviation.

In addition, Taylor dispersion analysis (TDA) is an absolute and straightforward characterization method from the size perspective for determining the diffusion coefficient, or equivalently the hydrodynamic radius. Chitosans were analyzed by TDA method and characterized by the full width at half maximum (FWHM) values of their signal peaks.

We managed thanks to those two methods to have a deeper characterization of chitosan samples with different FWHM but similar DA or with different DA but similar FWHM. Those chitosans were considered for preparing microparticles containing ibuprofen, thus allowing the establishment of structure-property relationships of chitosans in the oral controlled delivery.

Stabilization of Water-in-Water Emulsions by Complex Coacervate Core Micelles

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Poster 75

Keywords:

Water-in-water emulsions (WWE) form when aqueous solutions of incompatible polymers are mixed. These emulsions, that do not contain any organic phase, are of growing interest in soft matter due to their phase behavior and applications in encapsulation, separation and texturation. However, they possess a large interface and low interfacial tension, making the adsorption of molecular stabilizers, such as surfactants, difficult. Moreover, these all-aqueous systems require fully hydrophilic stabilizers displaying affinity for both phases (refered as bis-hydrophilicity). Therefore, using particles such as protein microgels or protein-polysaccharide complexes as stabilizers, namely Pickering effect, has proved effective in improving WWE stability. However, the relationship between chemical composition of the particles and their ability to stabilize WWE is poorly understood. A recent work showed that poly(ethylene oxide) (PEO)/dextran WWE in the presence of dextran-derived microgels displaying bis-hydrophilicity had an excellent stability. In this context, complex coacervate core micelles (C3Ms), consisting of polyelectrolyte complexes stabilized by a neutral hydrophilic polymer segment attached to one or both polyelectrolytes, appear as promising candidates. Indeed, their size and surface chemistry (thus, bis-hydrophilicity) can be tuned by varying the copolymer composition.
In this study, PEO/dextran emulsions in the presence of C3Ms with a PEO corona were developed. The role of the core in C3Ms partitioning will be highlighted. The ability of C3Ms to stabilize WWE varies with ionic strength.

Kinetic and Rheostructural Study of Hydrogel/Nanoparticle Double Networks Gelation

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Poster 69

Keywords: rheology ; silica ; nanoparticles ; sol ; gel ; colloidal gel ; PEGDA hydrogel ; gelation ; crosslinking ; small ; angle X ; ray scattering ; small ; angle neutron scattering ; mechanical properties ; structure

The synergistic effects of combining polymers and colloidal particles to create composite materials are well-known. However, the microscopic mechanisms behind these interactions, and the influence of the microstructure on the weakly non-linear rheology of composites, remain poorly understood. This is partly due to the experimental challenges posed by the structural complexity of mixing two materials with contrasted chemical nature and properties.

In this work, we develop a model double network system, composed of a colloidal gel made of silica nanoparticles interpenetrated with a poly ethylene glycol (PEG) hydrogel. Each network can be formed in controlled conditions to give reproducible structures and mechanical properties across a wide range of compositions. To finely explore the range of double network structures that can be obtained, we trigger the crosslinking of the polymer network during the aggregation of the colloidal gel. We then probe the time-dependent formation of the multiscale structure through a combination of X-ray and light scattering, and we relate it to the evolution of the linear viscoelastic moduli probed by rheology.

In a next step, rheostructural monitoring of the two-stage network build-up is taken as a basis for evaluating the gradual failure of the composites.

This work paves the way for a better understanding of the complex nonlinear rheology of composite materials, and its dependence on their microstructures.

Copper Embedded Ti-Metal-Organic Framework for Photocatalytic H2 Production from Formic Acid

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Poster 4

Keywords: metal ; organic framework ; hydrogen ; heterogeneous photocatalysis ; copper ; formic acid

Within the current environmental and energetic critical situation, finding more sustainable alternative energy resources has become a major challenge. In this regard, Metal-Organic Frameworks (MOFs) are considered as promising candidates. More specifically, Ti-MOFs are attracting more attention owing to their high promises as photocatalysts.
Among the Ti-MOFs family, MIP-177(Ti) is a phase-transformable titanium-carboxylate framework, exhibiting a dynamic structural adaptability and robust photoconductive properties. Its original form, MIP-177(Ti)-LT , is composed of Ti12O15-clusters interconnected by tetracarcoxylate linkers and decorated with formate ligands, while the thermal treatment induces the formate departure and, hence, the transformation of clusters to Ti-rods leading to the MIP-177(Ti)-HT. These MOFs have been shown to enable efficient electron-hole pair generation and separation under light irradiation. This resulted in exceptional photoconductivity, surpassing conventional TiO_2 systems by minimizing charge recombination and maintaining performance through structural transitions, as well as very promising photocatalytic performances towards producing H2 from water and from formic acid aqueous solution.
Building on these attributes, MIP-177(Ti) have been explored for photocatalytic hydrogen production from FA in vapor phase, a green hydrogen carrier with high volumetric capacity. While pristine MIP-177(Ti) predominantly follow the dehydration pathway (producing CO/H_2O) under UV light via Ti-oxo-units excitation, Cu-embedded MIP-177(Ti)s composites exhibit altered mechanisms. Indeed, post-metalation with Cu clusters (Ti/Cu $>$ 10 at%) shifts MIP-177(Ti)s towards the dehydrogenation pathway (producing CO_2/H_2) under both UV and visible light. Interestingly, while the amounts of Cu seem tuning the reaction pathway, the presence of Cu is very likely promoting a charge transfer enabling the photocatalytic activity under visible light. In this communication, we will present more in details the MIP-177(Ti)s and their peculiar features together with a specific highlight on their photocatalytic activity for H2 production from FA. Besides, the impact of Cu loading on the photophysical properties and catalytic mechanism will be also discussed.

From Self-Assembly to Formulation of Sustainable Surfactants

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Poster 58

Keywords: surfactants ; self-assembly ; SAXS

Surfactants from renewable resources are developed to replace petrochemical surfactants. Their attractiveness is explained by their biodegradability, low toxicity and their environmental friendliness but they are also known to present interesting solution self-assembly properties, controlled by temperature, pH or type of ion1.

However, some aspects are still challenging for a wider use of biosurfactants in industrial products, namely the high cost of production and the impact of purity on physico-chemical properties. Despite the control over the fermentation process, the crude extract is generally a mixture of several compounds composed of a majority of active matter and a fraction of water[2]. The active matter is composed of the biosurfactant and other molecules with close structure. Residues of fermentation are also found, with a non-negligible content of fatty acids.

Within this context, the goal of my PhD project is to understand the phase diagram of crude extracts of selected biosurfactants. The current state-of-the-art gives a wide range of CMC and surface tension values for the same molecules and a list of parameters such as temperature, pH, aging time, or concentration that could influence self-assembly properties. Identifying domains of stability and better understanding phase-transition conditions would ease the construction of phase diagrams by reducing the number of parameters involved. These phases can be determined by using X-ray scattering techniques. Once the phase diagram of the crude extract is built and the critical parameters for self-assembly identified, the impact of new components (co-surfactants, oils or salts) is studied to move towards more complex formulations and induce new properties.

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Chemical Analysis of the Königsfelden Stained Glass Windows: a pXRF Approach to Trace Their Origin

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Poster 44

Keywords: stained glass ; Switzerland ; pXRF ; LA-ICP-MS ; Optical spectroscopy ; Machine learning

The chemical composition and optical properties of the stained-glass windows in the Königsfelden Abbey church (Aargau, Switzerland), which are among the oldest and best-preserved examples from the 14th century in the region, were analysed on site using portable X-ray fluorescence (pXRF) and optical absorption spectroscopy. A subset of loose fragments was further characterised by Raman spectroscopy and LA-ICP-MS, and these data were used to improve the calibration of the results obtained with in situ pXRF. A machine-learning classifier (GLORIA) was applied to assess the variability of the glasses and their provenance relative to a reference database of European stained-glass windows. The results demonstrate that the Königsfelden corpus consists of potash-based forest glasses, mostly attributed to Central Europe (59%), with additional inputs from the Rhine region (32%) and Northwestern France (9%). While the colouring mechanisms for cobalt blue, copper red, manganese purple, silver yellow and iron sulphide amber are relatively well understood, the colouring techniques of a distinctive bluish grey and rare Pb-rich green glass (∼10 wt% PbO) are unusual and have no clear published parallels. One hypothesis for the high PbO contents in green glass is that a CuO-PbO frit was deliberately employed to facilitate the dissolution of metallic copper in the silicate melt. The blue-grey glass, unique in hue and composition, appears to result from the combination of a manganese–cobalt glass with an additional, yet unidentified, contribution. Our study thus provides new insights into medieval glass recipes, trade networks, and workshop practices, while also validating the potential of calibrated pXRF combined with reference standards and machine learning for heritage science applications.

From Solution-Processed Mesopores to More Efficient Perovskite Solar Cells

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Poster 80

Keywords:

Perovskite solar cells have attracted widespread attention in recent years due to their high efficiency and low-cost fabrication. However, the commonly used FTO conductive glass suffers from Fresnel reflection losses, with its transmittance typically limited to below 90%, thereby restricting light harvesting in devices. Inspired by the moth-eye structure, we fabricated nanopore arrays by solution-processes achiving different pore sizes and periodicities on FTO substrates to improve their optical transmittance. Experimental results demonstrated a significant enhancement in transmittance, with the best-performing sample exhibiting an increase of transmittance of approximately 27.4%. COMSOL simulations further validated the experimental findings and revealed that the enhancement originates from optical coupling and the gradual refractive index transition induced by the nanostructures. Based on this, the optimized nanostructure was integrated into functional perovskite solar cells, leading to both short-circuit current density and power conversion efficiency increases (ΔPCE $\sim$ +8.6%).

Self-assembly of biological systems: identification of collagen/apatite hybrid mesophases in bone tissue and for the diagnosis of related pathologies

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Poster 18

Keywords: Collagen ; Bone ; Mesophase ; Pathologies

Bone tissue ensures skeletal structure and function through dynamic remodeling of a complex matrix of mineralized collagen fibrils. Recent studies on sheep bone biopsies identified a deeper osteoid at the osteoid–bone interface, characterized by an acidic pH (∼5–6) and a collagen molecular organization distinct from fibrillar collagen. This acidic osteoid was described as a mesophase with continuous birefringence similar to mature bone, suggesting its role in the formation of the twisted plywood architecture. This work aims to characterize this domain in various bone pathologies.

To this end, we analyze physiological and pathological human biopsies together with collagen matrices mimicking the acidic osteoid. The synthetic osteoid is produced via an injection/dialysis process to elucidate the mechanisms underlying its formation. The collagen solution is supplemented with bone-relevant organic additives (glycosaminoglycans, citrate) and inorganic ions to induce carbonated apatite precipitation. In parallel, histological sections from human iliac crest biopsies with various pathologies were examined to characterize this domain in terms of density, composition, extent, pH, and organization. These investigations rely on an interdisciplinary approach bridging biology and materials science.

We show that in vitro models of the acidic osteoid domain can be synthesized in the presence of citrate and glycosaminoglycans. These additives stabilize a lower pH and induce differences in macroscopic, microscopic, and mineralization features. Analyses of pathological histological sections further reveal qualitative and quantitative destabilization of the acidic non-fibrillar domain in certain bone pathologies, also observed in adjacent mature bone. These findings suggest that mature bone organization directly depends on that of the underlying osteoid, which may contribute to pathological development.

This interdisciplinary work deepens our understanding of the physico-chemical processes governing bone formation and aims to validate a physico-chemical diagnostic approach complementary to anatomo-pathological and genetic analyses. These advances could open new avenues for

therapeutic development.

Stress relaxation in sol gel coatings during thermal tempering treatments – towards the development of new sustainable functionalities for glasses

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Poster 14

Keywords: sol ; gel ; revêtement ; contrainte ; verre ; diffusion ; nanoindentation ; Raman ; structure

Saint-Gobain's glazing incorporates numerous functionalities through coating application to address the thermal performance challenges of buildings and reduce their carbon footprint, for applications related to transportation or decoration. Since many glass products undergo thermal tempering (rapid annealing above the glass's T_g with rapid cooling by an air jet) – giving the glass greater mechanical strength – developing functional coatings resistant to high temperatures ($> 600°C$) is a significant challenge. Sol-gel coatings are particularly promising candidates to address this issue. Their inorganic nature, obtained through chemical reactions of hybrid precursors, provides them with good temperature resistance and ensures strong covalent adhesion to the glass substrate. Furthermore, the wide variety of precursors available on the market allows for a broad range of compositions and therefore diverse properties (refractive index control coatings, colored coatings, scratch-resistant coatings, etc.). However, several effects occur during the drying, annealing, and cooling stages of the sol-gel on glass. These include solvent evaporation, lattice condensation, thermal expansion, and ion diffusion from the substrate. These cumulative effects create high stresses that generate cracks in the layer. The first part of my thesis was dedicated to investigating the reasons and chronology of the appearance of these phenomena, as well as their consequence on the mechanical properties, structure and stresses developed in the layer.

Synthesis of new catalytic materials under high pressure

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Poster 73

Keywords: high pressure ; synthesis ; catalysis ; novel materials

High pressures are a powerful tool to synthesize novel materials, providing pathways inspired by Earth's own geological processes [1]. By inducing phase transitions, they enable the stabilization of structures and access the formation of compounds that are unattainable under ambient conditions [2].

One of the key advantages of high pressures is to limit grain growth, thereby enabling the recovery of nanostructured with drastically enhanced properties. This principle has been demonstrated in ultra-hard materials like diamond [3] and cubic boron nitride [4]. Beyond hardness, the combination of high pressures and nanostructuration is a promising route to tailor functional properties related to the nanoscale. Indeed, at the nanoscale, several materials exhibit enhanced properties such as magnetism, charge transport, and catalytic properties, as evidenced by transition metal silicides [5,6] and boron-based compounds [7].

In this presentation, we present the synergistic impact of high pressures and nanoparticle engineering on the development of advanced catalytic materials. Our focus will be set up on materials for hydrogen production through water splitting and for CO2 valorisation into high added-value molecules. Using high-pressure synthesis, in situ XRD measurements and various structural characterization, we are able to design new catalytic compounds. An emphasis is placed on compounds of transition metals with silicon and boron, highlighting new catalytic phases, their structural evolution under pressure and their potential applications in energy and environment-related technologies.

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Confinement of Tamm modes in the THz spectral range

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Poster 1

Keywords: terahertz ; cavities ; photonics ; bragg reflectors ; resonators ; confinement ; quality factor

We report on the confinement of THz Tamm modes in 0D Tamm cavities consisting of a finite-sized metallic disk deposited on a distributed Bragg reflector. Reflectivity spectra measurements reveal high quality factors of 490 and 310 for 0D Tamm cavities resonating at 308 GHz and 684 GHz, respectively. Both experimental results and theoretical analysis demonstrate the confinement of the Tamm modes in all three spatial dimensions. The modal dispersion relations of Tamm 0D cavities, measured using an angle-resolved spectroscopy experiment, exhibit discrete energy modes in contrast to the parabolic dispersion relation measured for a Tamm 2D cavity. Electromagnetic simulations show the lateral confinement of the Tamm mode beneath the metallic disk. These 0D Tamm resonators hold great potential for ultra-strong coupling to 0D quantum systems, such as artificial atoms or molecules.

Nanoscale control of heat flux in self-assembled ordered nanocrystal solids

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Poster 28

Keywords: heat ; thermal ; transport ; nanocrystals ; superlattice ; anisotropy ; gold ; nanorods ; monolayer

Nanocrystal-based solids represent a versatile class of materials whose collective properties can be finely adjusted by tuning parameters such as shape, size, chemical composition, and surface ligands. These materials are particularly relevant for advancing plasmonic, optoelectronic, and thermoelectric technologies. Controlling thermal transport within such systems is crucial, as local heating—whether induced by optical absorption or electrical current—can impair performance, cause instability, or trigger undesirable reactions. In this contribution, I will discuss recent findings on the heat transport properties of superlattices composed of gold nanospheres, nanorods, and nano-bipyramids. Using correlative scanning electron microscopy and spatio-temporally resolved thermoreflectance techniques, we accessed thermal dynamics with nanosecond resolution and sub-micron spatial detail. In polymer-ligand-capped gold nanosphere assemblies, we observed that monolayer configurations exhibit faster thermal diffusion compared to multilayers. Monte Carlo simulations incorporating quasi-ballistic phonon transport suggest this behavior arises from the interplay between extended phonon mean free paths and ligand interdigitation. In assemblies of gold nanorods and bipyramids, our results show that heat preferentially propagates along the nanoparticles' longitudinal axis, maintaining directional flow even in bent or curved configurations. In ordered superlattices, this results in pronounced anisotropic heat conduction, with higher diffusivity along the particles' elongation. Finite element analysis and effective medium theory confirm that this directional transport can be tuned by modulating particle shape, aspect ratio, and packing geometry. Harnessing such anisotropy offers new strategies for improving heat dissipation and directing thermal flow within functional devices, all while preserving tunable optical and electronic properties.

Hydroxyapatite-supported Ru Catalysts for the chemical Storage of H2 as Ammonia

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Poster 2

Keywords: Ammonia synthesis ; Hydroxyapatite ; Ruthenium catalyst ; Electron density ; Turnover frequency

Ammonia (NH_3) is the second most produced chemical in the world, mainly used for fertilizer production and now emerging as a promising energy carrier. Its conventional synthesis via the Haber Bosch process is highly energy-intensive and generates large amounts of CO_2, motivating the search for more efficient catalytic systems.

In this work, Ru-based catalysts supported on hydroxyapatite (HAp: $Ca_{10}(PO_4)_6(OH)_2$) were developed and investigated for the catalytic synthesis of ammonia. HAp supports were prepared by coprecipitating $NH_4H_2PO_4$ and $Ca(NO_3)_2$ solutions at 80°C and at different pH values, then impregnated with 2 wt% Ru using a $Ru(NO_3)_3$ precursor and reduced under H_2 at 450°C. The Ru/HAp catalysts precipitated at pH values between **7.4 and 7.8** exhibited the **highest ammonia synthesis performance** at 400°C and 1 bar, with a turnover frequency (TOF) of 0.40 ± 0.01 min^{-1}, approximately 50% higher than that of a Ru/MgO reference catalyst.

TEM analysis showed Ru nanoparticles with an average size of 2.2 ± 0.2 nm on HAp, slightly smaller than those on MgO (2.4 nm). The enhanced catalytic activity was strongly correlated with the electron density of Ru nanoparticles, as revealed by FTIR measurements of adsorbed N_2 (εN_2–Ru0). The results suggest that the rate-determining N_2 dissociation step is promoted by electron transfer from the Ru d-orbitals to the π^* antibonding orbital of N_2. The high performance is attributed to the basicity and defect structure of HAp, which stabilize electron-rich Ru sites. This work demonstrates hydroxyapatite as a promising support for Ru catalysts in ammonia synthesis.

Synthesis and cell-interactions of polynucleotides-based dynamic nanoparticles for gene delivery applications

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Poster 24

Keywords: nanoparticles ; polyoxazolines ; lipid membranes ; gene therapy

Gene therapy involves introducing polynucleotide-based drugs into specific cells to modulate cellular activity for therapeutic purposes. For plasmid DNA-based delivery, tracking toward and into the nucleus of the targeted cells requires the use of a vector. Currently, recombinant viral vectors such as adeno-associated virus (AAV) offer the highest transfection efficiency. However, costly large-scale production of these vectors and their potential immunogenic risks, make the exploration of non-viral vectors an appealing area of study. The use of polymers is an alternative to overcome viral issues: it has been demonstrated that polycations can efficiently condense pDNA into particles at the 100 nm scale for dilute solutions. These large particle sizes, combined with the intrinsic toxicity of cationic polymers, lead to toxicities that are incompatible with therapeutic development.

In this project, we develop a library of 3 and 4 arms star PEI in a 2 steps procedure to overcome some of the toxicities issues: a 1st step of cationic ring opening polymerization (CROP) to synthesize star poly(2-ethyl-2-oxazoline) and a 2nd step to reveal the ethylenimine backbone through acidic hydrolysis. The polymers structures are characterized by 1H, 13C, COSY, HSQC, DOSY NMR and the molar masses are evaluated by SEC.

To assess the molecular mechanism ruling polycations and/or polyplexes interaction with cell membranes, associated with their toxicity linked, for example, to excess of positive charges, we designed a set of biophysical experiments exploiting Langmuir films. The cellular interface is mimicked by lipid films of variable composition deposited at the air-water interface, and the effects of polymers on their stability and compactness are investigated. Results indicate that

a correlation between toxicity and cationic polymers nature can be attempted and, notably, indicate that with interdisciplinary approaches as our, pDNA transfection efficiency can be tuned and increased.

Study of MOFs (Metal-Organic Frameworks) for H/D/T Isotopic Separation

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Poster 31

Keywords: MOFs ; hydrogen ; isotopes ; separation

The tritium content of some waste from CEA's activities makes it incompatible with the environment and must therefore be separated from the rest to decontaminate the light elements. To accomplish this separation, zeolites are currently used in CEA. Those materials are reported in the literature as the benchmark for this application, particularly some chabazites

To find an alternative to zeolites with improved performance, Metal-Organic Frameworks (MOFs) are considered as promising candidates. They are highly versatile in terms of applications, thanks to their diverse structures and their various physicochemical properties, which can be finely tuned and on purpose. Among the various separation mechanisms, two are typical for hydrogen isotope separation ($H_2/D_2/T_2$). The first, known as 'Kinetic Quantum Sieving' (KQS),is based on kinetic separation induced by confinement in small pores with diameters close to those of H_2 and its isotopes. The second, 'Chemical Affinity Quantum Sieving' (CAQS) enables isotopic separation thanks to different chemical affinities between the adsorbent and the adsorbate, particularly on strong adsorption sites such as Open Metal Sites. As part of this collaborative project between IMAP, CEA Valduc and ICB, we are relying on these two separation mechanisms to guide our choices to find high-performance MOFs combining both high selectivity and adsorption capacity.

In parallel, some preselected MOFs (covering various chemical and structural features) will undergo radiation tests to assess their stability under beta radiation from the tritium present in small quantities in the gas mixture to be treated. These tests will mimic a representative environment of real-life conditions, which is an essential criterion to select the most appropriate sorbent for this application.

Thus, this presentation will introduce the work developed within the frame of this project, the various aspects of hydrogen isotope separation, and provide an overview on benchmark sorbents for hydrogen isotopic separation, including some reported MOFs.

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Growth dynamics of irregular eutectics: in situ experiments

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Poster 27

Keywords: Directional solidification ; in situ observations ; aluminium based alloys ; irregular eutectics ; thin ; sample ; impurities ; Fe ; IMs ; dual ; scale optics

In order to conform to EU climate goals, the aluminum industry promotes a circular economy via the substitution of primary aluminum with post-consumer scrap, thus achieving substantial energy savings. Unfortunately, impurities such as iron and silicon are present in an increasingly large amount in recycled materials.This increases the volume fraction of Fe-rich intermetallic (IM) precipitates that impact negatively the final formability properties of wrought aluminium alloys. Instead of attempting to eliminate those IMs, an engineering strategy consists of intentionally using addition elements that modify the nature and the shape of the IM phases, and decrease their detrimental effect. The physical processes at play are, however, not fully understood. My PhD work aims to investigate experimentally the nucleation and growth dynamics of Fe-rich IMs in model multi-component alloys such as Al-Si-Fe and Al-Si-Fe-Mn. In-situ observations using an original dual-scale optics are performed during directional solidification of thin (10 μm thick) metallic films in a well-calibrated temperature gradient. This method provides real-time access to the solidification dynamics of both primary and secondary IMs in interaction with the growing Al matrix over a large range (0.1—100 μm/s) of the imposed growth velocity V. By this way, we achieved the first in situ observation of a morphological transition from faceted growth of individual IM crystals to coupled growth of the IM-Al irregular eutectic as a function of V. Additional information is given by ex situ chemical and crystallographic characterization of the different solid phases. The analysis of the observed phenomena is made in reference to solutal-diffusion and interfacial-kinetic effects, with the help of thermodynamic calculations.

Synthesis, Characterization, Electrochemical, Optical and Magnetic Properties of New Members of the $Li_2M_2W_2O_9$ (M = Mn, Fe, Co) Family

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Poster 65

Keywords: synthesis ; crystallography ; lithium ion batteries ; electrochromism ; magnetism

The relentless quest for new electrode materials for energy storage and electrochromic devices remains essential to improve current technology. Building on our previous discovery of $Li_2Ni_2W_2O_9$ – a corundum-like compound with reversible Li^+ intercalation and electrochromic behavior – we report three new phases – $Li_2Mn_2W_2O_9$, $Li_2Fe_2W_2O_9$ and $Li_2Co_2W_2O_9$ – synthesized via ceramic and carbothermal reduction methods. The three phases crystallize in either the orthorhombic Pbcn or the trigonal P c1 space groups and feature cationic mixing between the 3d-transition metal (Mn, Fe or Co) and Li at varying levels. These materials were characterized to investigate their unique structural features, electrochemical behavior, optical response and magnetic properties. Operando optical reflection microscopy revealed distinct light-matter interactions: $Li_2Fe_2W_2O_9$ and $Li_2Mn_2W_2O_9$ showed contrast changes due to volume change during Li^+ (de)intercalation, while $Li_2Co_2W_2O_9$ exhibited dual optical responses dominated by either light absorption or volume change. This approach enabled us to probe and comparatively rank electrochromic efficiency across the series as: $Li_2Ni_2W_2O_9 > Li_2Co_2W_2O_9 > Li_2Mn_2W_2O_9 >> Li_2Fe_2W_2O_9$. Magnetic characterization uncovers long-range antiferromagnetic ordering in both $Li_2Fe_2W_2O_9$ and $Li_2Co_2W_2O_9$, with magnetic structures proposed in the *Pbc'n* and refined in *Pb'c'n* Shubnikov space groups, respectively. This comprehensive study reveals how transition-metal chemistry governs the interplay between electrochemical, optical, and magnetic properties in the $Li_2M_2W_2O_9$ family, offering a tunable platform for future multifunctional en-

ergy materials.

Understanding rare-earths environment for better mechanical properties in reinforcing fiberglass

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Poster 10

Keywords: glass ; fiber ; structure ; properties ; rareearths ; exafs ; nmr ; raman ; synthesis ; hot

As energy demands increases, the need for evermore efficient wind turbines arises. To answer those needs, materials need to be lighter, stronger, cheaper and paramountly, more resistant. Fiberglass composites have been used for decades as it meet all those criteria. Where polymer resins bring chemical resistance, it encases fabrics of woven fiberglass that brings rigidity and structural resustance. It is thus those fiberglass that must be improved and made more resistant. Studies have shown an increase of Young's modulus by a more compact structure[1] either through rare-earths (RE) oxides addition[2] or through alkaline and alkaline-earths oxides. As yttrium and lanthanum are often considered oxides of interest for stronger glasses, the effect of the addition of a few molar percents of those oxides was studied on a simplified industrial composition.

Synthesised glasses were studied through ^{27}Al NMR spectroscopy, Raman spectroscopy, K-edge EXAFS spectroscopy of yttrium and lanthanum as bulk and fiberized samples. It has thus been shown that rare-earths increases the population of highly-coordinated aluminium (5- and 6-fold coordinated Al). This increase in reticulation ought to increase compacity and thus rigidity[2]. However, whereas yttrium increases Young's modulus, lanthanum has close to no effect on this parameter. This difference has been studied through EXAFS and molecular dynamics to understand the differences in local environmnent of rare-earths in the $MgO - Al_2O_3 - SiO_2$ matrix. It has notably been shown that yttrium is mainly 6-fold coordinated where lanthanum is mainly 8-fold coordinated.

Switable cavitation in soft matter

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Poster 76

Keywords: soft matter ; cavitation ; pores ; elasticity ; finite element ; simulations ; polymers ; gels

Stimuli-responsive buckling, wrinkling and creasing on the surface of soft polymers and gels can be used for design of self-assembled materials and sensors and have been intensively studied in the literature. Recently, similar phenomenon have been explored in non-flat geometries, for example on a surface of a spherical cavity within an elastic solid. Moreover, a new phenomenon of reversible opening/closing of small spherical cavities was observed and has potential applications. In a possible explanation, a soft pore (Figure 1. a) may be bistable (i.e., may remain an infinite amount of time in both closed and open state) due to the competition between the adhesion energy of inner surfaces of the cavities and the strain energy inside the matrix. However, the role of surface instability and of interfacial interactions remains poorly understood.
In this work, we performed finite element simulations and experimental investigation of compression of model soft pores. On the Fig 1.a, we show the total energy of a 2D pore in a neo-Hookean elastic matrix with an adhesive contact between the pore walls as a function of the normalized contact surface A_{closed}/A_{total}. By varying the ratio (E*R)/γPDMS, where E is Young's Modulus, R is the initial radius of the pore, γPDMS is the surface energy of the matrix, we demonstrated the bistable behavior at intermediate values of R. When R is small, the Etotal decreases with A_{closed} which means the pores will spontaneously collapse. For large pores, the release of the external force will lead to reopening of pores. In experiments, isolated pores inside a soft PDMS matrix were fabricated via emulsion technique and the sample was compressed (Fig 1.b): we show that pores remain closed after the force is released which is due to the adhesive force.

Synthesis of well-controlled amorphous vitrimers

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Poster 21

Keywords: Polymer chemistry ; organic chemistry ; vitrimers

The aim of the project is the use of fine synthetic procedures to exercise control over different parameters in dioxaborolane-based polystyrene, polymethacrylate and polyacrylate vitrimers, in order to study the impact of these on their properties. The procedure is to start with the synthesis of a functional monomer possessing chemical groups capable of dynamically exchanging and then copolymerize it via different polymerization methods with a commercial monomer. Once a fully thermoplastic vitrimeric precursor has been obtained, it is possible to insert in different quantities a cross-linking agent with dynamic reactivity towards the pendant groups present in the polymer, thus producing a vitrimer.

Understanding the varieties of obsidian: insight into the compositional and structural characteristics

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Poster 38

Keywords: obsidian ; redox ; XAS ; color ; viscosity ; volatiles

Owing to their high silica (∼70 wt%) and alumina (>10 wt%), obsidian exhibits high viscosity, melting point and glass transition temperature. More crucially, it includes a low but significant amount of volatile components, primarily water (typically <1 wt%), whose degassing process influences the quenching of the lava. The final glass may or may not contain bubbles and/or crystallized phases, mainly of iron, in the form of nanolites. Typically, the iron content of obsidian does not exceed 2 wt% often only half as much. It is iron that determines the color of the glass. Although obsidian is often associated with a characteristic deep black colour, it can in fact exhibit a great variety of colors, including red, brown, grey, deep blue, and green. This variety is not necessarily the result of different geological processes or chemical compositions, as different obsidians often occur in close proximity of each other. The coloration mechanisms vary: black hues arise from iron-rich nanolite clusters, while the red color is linked to dispersed iron oxide microcrystals. The remaining colors are still a matter of debate.

To better understand the complex processes that contribute to the formation and diversity of obsidian, we investigated the composition and crystalline structures of several kinds, mainly of black and red varieties. Specifically, several analytical methods were employed (e.g. EPMA, XAS, Raman spectroscopy, viscosity measurements) to explore the nature of the nanolites, water contents and viscosity to better understand the effect of water in the glass and the iron speciation in both crystals and glass.

Industrial Feasibility of Capacitive Salinity-Gradient Energy Systems: Optimization for High Power Density

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Poster 47

Keywords: Blue energy ; CRED ; RED

CRED (Capacitive reverse electrodialysis) cells are a hybrid technology that were originally introduced by Vermaas to extract electrical energy from salinity gradient[1]. They use selective IME (ion membranes exchange) just like RED (Reverse Electrodialysis) systems but borrow long-lasting, non-faradaic and inexpensive capacitive electrodes from Capmix (Capacitive Mixing) systems achieving power densities around 0.9 W/m² of IME, 5 times higher than Capmix systems[2] but 2 times lower than RED systems[3].

The current system designed only uses one IME and carbon felts as capacitive electrodes. The whole cell is equivalent to an ideal generator Ecell, an internal resistance Rcell and an internal capacitor C in series. Due to the internal capacitor, the cell must be used in an alternative regime by switching the concentrated and diluted solutions of sodium chloride over a switching-period T. The uptake of these 3D electrodes increases drastically the capacitance allowing us to achieve around 2.3 W/m² by stabilizing the potential; which can even reach 3.3 W/m² by choosing an appropriate half-period and reducing the internal resistance by employing thinner membranes and higher concentrations[5].

The initial strategy involves the industrialization of the CRED cell by enlarging the surface area of individual membranes. Particular attention will be given to the impact of increasing the membrane length (along the flow direction) and width. The extension of the length highlights the problem of the filling time that has to be as short as possible in order to reach the maximal potential as quick as possible and approach a square signal while not having too much viscous loss. Increasing the surface of one membrane helps reducing the total inner resistance of the cell resulting in a higher current. We will then associate in series CRED cells to obtain cumulative potential and power while preserving power density building bigger and compact cells.

Development of self-healing and recycled hybrid dynamic networks

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Poster 37

Keywords: self-healing ; polymer ; hybrid networks ; recycled ; dynamic ; mechanical properties

In 2022, the global annual production of polymeric materials reached 400 million tons, and demand continues to rise. The development of self-healing materials represents one of the promising approaches to reducing plastic consumption. Such materials can extend the lifetime of polymers and help limit waste generation. Indeed, polymer materials age and degrade over time, leading to a loss of functionality and a decrease in some of their properties, particularly their mechanical performance. To compensate for these losses, and among the strategies developed to enhance material durability, this class of self-healing polymers—capable of repairing themselves when exposed to a stimulus such as temperature—aims to recover the initial properties of the material, including mechanical strength and elongation at break. A self-healing material is also less likely to experience irreversible damage, which significantly improves its durability. Furthermore, following an approach based on the design of polymer networks with dynamic properties, new hybrid composite materials are proposed by combining polymers with an inorganic component. To develop these composite materials, oxide particles functionalized with various organic groups via a sol–gel process are introduced and dispersed into the molten polymer. The impact of the inorganic component within the organic matrix on mechanical properties (Young's modulus, elongation, and stress at break), as well as on the self-healing, shape-memory, and recyclability properties of the polymer, will be discussed.

Dynamic viscoelastic response of nanoscale interfacial water on lamellar materials

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Poster 48

Keywords: Confined water ; Viscoelasticity ; Nanorheology ; Hydration layers ; Yield stress fluids ; Atomic force microscopy ; Interfacial dynamics ; Nanoscale friction

Water under nanometric confinement displays remarkable deviations from bulk behavior, yet its viscoelastic nature remains debated. Using dynamic atomic force microscopy operated in both normal and tangential modes, we probe the mechanical impedance of water confined between a tungsten tip and atomically flat substrates of contrasting hydrophilicity: mica, highly oriented pyrolytic graphite (HOPG), and hexagonal boron nitride (hBN).

At low confinement, the interfacial water behaves as a shear-thinning fluid dominated by dissipation. At higher confinement, it undergoes a transition to a yield-stress regime, where elastic and viscous contributions become comparable. The intrinsic relaxation timescales extracted from viscoelastic modeling reveal a massive slowdown—up to seven orders of magnitude compared to bulk water—corresponding to effective viscosities of 10–100 Pa $\cdot$ s. Within this framework, the effective modulus lies in the MPa range, suggesting nanometric correlation domains and slow structural relaxation reminiscent of supercooled water.

Both the yield force and critical shear amplitude increase with confinement, revealing a strong dependence on surface hydrophilicity: interfacial water on mica resists flow more strongly than on HOPG or hBN. We attribute this behavior to an increase in the effective corrugation potential and to a shift of the relaxation plane toward the hydrophobic surface in asymmetric confinements.

Altogether, our findings provide a unified picture of confined water as a slowly relaxing, viscoelastic medium bridging the behaviors of bulk liquid and and supercooled water. This framework not only reconciles previous discrepancies in reported viscosities but also sheds light on interfacial transport and nanofluidic friction at the solid–liquid interface.

Friday, November 14th

Eco-responsible synthesis of heterogeneous catalysts via a solvent-free sol-gel approach

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Poster 55

Keywords: solgel ; sustainable catalysts ; solventfree ; zirconia

Catalysts are indispensable in today's world. While they enable more sustainable chemical transformations, it is equally important to consider the environmental impact associated with their production. Although various methods exist for producing heterogeneous catalysts, most of them have adverse environmental consequences as they rely on solvent-intensive protocols and generate waste.

In this study, we present a solvent-free sol-gel strategy for the synthesis of oxide and mixed oxide-based catalysts. This single-step, waste-free, and continuous approach eliminates the need for solvents, significantly reducing the environmental footprint of catalyst production.

Haddad et al., used this approach for the preparation Ru-doped γ-Al_2O_3. Yet this approach was not tested for alkoxides with higher reactivity and also for mixed oxides. So, we wanted to make the solvent-free sol-gel strategy, a toolkit for the synthesis of sustainable heterogeneous catalysts. The approach has been successfully utilized for the synthesis of ZrO_2 and CeO_2-ZrO_2 systems.

A highly reactive zirconium isopropoxide was chosen as the zirconium precursor and its reactivity was lowered by varying the ratios of acetylacetone (acac) which is a bidentate chelating ligand. Cerium acetylacetonate ($Ce(acac)_3$) was chosen as the cerium precursor and the ratio of acac/Zr was varied and its impact was studied. Various doping concentrations of CeO_2 including 5 mol%, 10 mol% and 14 mol% have been successfully synthesized. XRD revealed the presence of pure tetragonal phase of ZrO_2 with no impurities. The peaks shifted towards lower 2Θ with an increase in doping concentration of CeO_2. The HAADF-STEM images represent a homogeneous distribution of CeO_2 over the ZrO_2 matrix. The surface area was found to be 50-80 m^2/g depending on the doping concentration and the acac ratio. The synthesized catalysts were tested for the ketonization of acetic acid. The catalysts showed 100% selectivity towards acetone and had a better performance than the commercial ones.

Ultra-broadband THz Emission from One- and Two-Color Laser-Induced Microplasmas at High Repetition Rate

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Poster 15

Keywords: Terahertz ; plasma ; femtosecond lasers ; time domain spectroscopy

Electromagnetic radiation in the terahertz domain (1 THz = 10^{12} Hz $\sim$ 4 meV) is widely used to conduct condensed matter study of meV excitations in spectroscopy experiments. Producing THz radiation has historically been a challenge because very mature technologies from photonics and electronics have shown to be highly inefficient when applied at THz frequencies. New kinds of emitters and detectors have been developed to overcome this challenge. The most popular sources today are based on photoconductive antennas or optical rectification in non-linear crystals, but their bandwidth (0.1 – 4 THz) and electric field amplitude (100 V/cm) are limited by their solid-state nature.

Using powerful femtosecond lasers, it is possible to attain intensities high enough to ionize air molecules and form plasmas that emit THz radiation. These plasmas are a promising tool to increase THz bandwidth and amplitude in spectroscopy experiments. However, plasma generation is mainly done with strong pulses ($\sim$mJ) from lasers at low repetition rate (1 kHz), which results in low signal to noise ratio (SNR). Our project aims to develop a new approach using Ytterbium fiber laser operating at MHz with µJ pulses. It is still possible to obtain high intensities above ionization threshold by using strong focus with high numerical aperture optics. This results in a micro-plasma with dimensions below 100 μm (Fig 1.a).

Along with one-color plasmas, we studied a two-color configuration where a mix of fundamental laser wavelength and its second harmonic is used for plasma generation. We observe an increase of the conversion efficiency by two orders of magnitude with the two-color plasma, resulting in broadband (0.1 – 30 THz) and powerful ($\sim$100 kV/cm) THz pulses (Fig 1.b). We also studied properties of the emission to guide theorical work aiming to extend accepted THz generation mechanisms in long plasmas to the μ-plasma geometry.

Quantification of Color Change for Polydiacetylene-Based Sensors

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Poster 41

Keywords: Soft matter ; Langmuir films ; Polydiacetylene ; Polymerization ; Fluorescence ; Synchrotron ; X-rays

Polydiacetylenes (PDAs) are a family of smart conjugated polymers known for their striking color and fluorescence changes—from blue to red—when exposed to external stimuli such as temperature, light, or mechanical stress. Owing to these unique properties, they are considered highly promising materials for developing sensitive optical sensors. The overarching objective of this work is to quantitatively correlate the chromatic and fluorescence transitions ("off–on" behavior) with the degree of external stimulation. In this study, we developed ultra-thin PDA-based films (approximately 5 nm thick) functionalized with fluorescent tetrazine groups. These films were precisely organized at the air–water interface using the Langmuir film technique. Their structure and properties were characterized using a combination of techniques : synchrotron Grazing Incidence X-ray Diffraction (GIXD) to probe molecular organization, X-ray Reflectivity (XRR) to determine average film thickness, Atomic Force Microscopy (AFM) to study surface topography, and UV–Visible absorption spectroscopy to monitor the polymerization process. We found that the molecular organization within the films strongly influences their polymerization behavior and optical response. Depending on the molecular structure, the resulting films exhibit distinct supramolecular organizations and polymerization efficiencies, which in turn lead to variations in their chromatic intensity and stability. These findings demonstrate how molecular design and film organization dictate the optical response of PDA-based systems, paving the way toward quantitative, ultra-thin sensors capable of visually detecting and measuring subtle environmental changes.

New sustainable polymer derived from reaction of thiolactone and cyclocarbonate

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Poster 29

Keywords: sustainable polymer; thiolactone

A key challenge in developing next-generation sustainable materials lies in designing polymers that can be easily converted back to their starting monomers via chemically recycled monomers (CRMs).[1][2] Introducing sulfur atoms into the polymer backbone enhances polymer properties in many areas, including improved mechanical, optical, and thermal properties, as well as metal ion adhesion. These enhanced properties make sulfur-containing polymers highly promising polymeric materials [3]. Emma et al., for the first time, used a benzyl alcohol-phosphazene base as an initiator system to systematically study the ring-opening copolymerization of γ-thiobutyrolactone and ethylene carbonate. The polymer has applications in nanotechnology and various biomedical fields.

In this work we developed a novel "depolymerization-oxidation-polycondensation" strategy: First, the polymer is completely depolymerized into monomers using a NaOH/meth- anol/THF system. Subsequently, the sulfur atoms are controlled and oxidized at the molecular level to yield monomers containing sulfoxide or sulfone functional groups. Finally, a polycondensation reaction generates polymers with novel structures and functions. This cyclic process have great significance for promoting green materials and sustainable development.

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Synthesis and characterization of new self-assembled thermally activated delayed fluorescence (TADF) molecular materials

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Poster 11

Keywords: Self-assembly; Liquid crystal; Exciplex; TADF; Optoelectronics

Since 2012, research on thermally activated delayed fluorescence (TADF) emitters has attracted considerable attention for light emitting device applications such as OLEDs.These molecules can convert up to 100% of the electrical excitations into light by harvesting both singlet and triplet excitons, without requiring expensive heavy metals as is the case for phosphorescent materials. Various molecular designs based on donor-acceptor architectures have been developed to achieve TADF, including exciplex systems. Such bimolecular systems enable efficient separation between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), which is known to promote TADF. In this project, we have chosen to develop a new approach that combines exciplexes with liquid-crystals (LCs). More precisely, we focus on donor-acceptor (D-A) discotic mesogens combining a reported discotic electron donor based on a triindole core and a new discotic electron acceptor based on triazatruxene core interacting through space within supramolecular arrangements. The use of such anisotropic systems as emitting layers should offer optimized light out-coupling efficiency, which is dependent on the orientation of the transition dipole moment (TDM) of the emitting molecules. The emission of light being predominantly in a direction perpendicular to the TDM, controlling the orientation of luminescent molecules in the emissive layers is an interesting approach to enhance the global efficiency of the devices.

Preliminary results obtained from polarized optical microscopy, differential scanning calorimetry, and fluorescence spectroscopy support exciplex formation. More particularly, a significant redshift of the emission spectrum is observed when comparing the neat donor film to the blends of the donor and the acceptor, which is known to be indicative of exciplex formation. Complementary experiments of time-resolved spectroscopy will be performed to confirm this statement.

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Biosourced archeomimetic pigments

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Poster 35

Keywords: Pigments ; dyes ; archeomimetic ; materials ; heritage conservation ; cosmetic

Colour has always been a means of expression for centuries, and depends heavily on the interaction between light and matter. In this context, inorganic pigments are the most widely used due to their photostability. Throughout history, hybrid pigments have also been created in an attempt to combine the advantages of inorganic materials with those of organic dyes, as demonstrated by the Maya blue[1], which is made from a clay (palygorskite) and indigo, and later by lake pigments made from alum and alizarin. They offer more intense and original colours, but are photosensitive.

It is in this context that this thesis fits in, by combining organic matter (dyes) and inorganic matter (clays, metal cations). Environmental considerations and sustainable development have been considered throughout this work.

Initially, lake pigments were synthesised using an archaeomimetic approach, forming oxyhydroxides based on betanin[2], a dye extracted from beetroot, and cationic salts of zinc, aluminium or copper. In a second stage, work continued on developing hybrid pigments using the same dye combined with modified clays[3], as well as using another natural dye, anthocyanins from grapes, to make new pigments.

These pigments were analysed using several characterisation techniques: X-ray diffraction (XRD), Fourier transform infrared (FTIR) vibrational spectroscopy, X-ray fluorescence (XRF) spectrometry, transmission electron microscopy (TEM), ssNMR and UV-VIS reflectance spectroscopy, as well as thermal analyses (TGA).

The most chemically stable pigments were subjected to accelerated ageing under a xenon lamp to study their photostability, with a purpose of applications in cosmetics or heritage conservation, such as the restoration of art paintings or masterpieces.

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Conception, Synthesis and Characterization of Hybrid Membranes for Proton Exchange Membrane Fuel Cells

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Poster 61

Keywords: PEMFC; membrane; polymer; hybrid; electrospinning

In response to growing environmental challenges, the European Commission has set the objective of achieving carbon neutrality by 2050 and accelerating the development of green hydrogen. Essential to energy transition, fuel cells facilitate the deployment of hydrogen-powered vehicles. In this context, this work focuses on developing organic-inorganic hybrid membranes for Proton Exchange Membrane Fuel Cells (PEMFCs), targeting high performance under elevated temperatures and low humidity. Commercial membranes often fail under such conditions due to poor mechanical stability and reduced proton conductivity.[1]

This PhD project investigates functionalized hybrid membranes synthesized through sol-gel chemistry and electrospinning. Poly(vinylidenefluoride-co-hexafluoropropylene) (PVDF-HFP) was employed as the organic matrix for its relative low-cost, high performance and ease of processing. To enable proton conductivity through sulfonic acid groups, silica precursors were introduced to form the inorganic network. Electrospinning enabled the creation of an interpenetrating organic-inorganic network, which effectively prevented phase separation between components.

By optimizing both the formulation and electrospinning parameters, uniform and well-controlled fibers were obtained, leading to enhanced conductivity and mechanical properties. Subsequent densification by hot-pressing further improved mechanical strength and ionic transport. Some membranes achieved proton conductivities up to 10^{-1} S/cm at 80°C and 80% RH, while maintaining stable mechanical properties with increasing temperature. Other strategies, such as impregnation of hybrid electrospun membranes, were also explored to reduce hydrogen crossover and enhance overall performance.

These results demonstrate a scalable and versatile approach for fabricating high-performance hybrid membranes, paving the way for their integration in PEMFC applications.

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Modeling the Mode of Action of Biopolymers and Amino-Molecules for the Protection of Earthen Constructions

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Poster 57

Keywords: raw earth; biopolymers; swelling

Earthen construction provides an environmentally sustainable alternative to conventional building materials thanks to the abundance, recyclability, and low carbon footprint of clay. However, the high water sensitivity of clay remains a major limitation: fluctuations in humidity induce swelling–shrinkage cycles that lead to cracking and structural failure. Among clay minerals, montmorillonite—a smectite with a 2:1 layered structure—is particularly prone to swelling, as its interlayer space can incorporate water through hydration of exchangeable cations.

Previous studies have shown that amine-based polymers can both suppress swelling and improve mechanical strength [1]. To elucidate their mechanism of action, this study investigates simpler alkyl-α,ω-diammonium compounds as model swelling inhibitors for montmorillonite. In aqueous clay suspensions, the protonated amine groups can exchange with interlayer cations, while the hydrophobic alkyl chains restrict water ingress [2][3]. The efficiency of three diamines — 1,8-diaminooctane (DC8), 1,10-diaminodecane (DC10), and 1,12-diaminododecane (DC12) — was examined at varying fractions of the clay's cation exchange capacity (CEC).

Crystalline swelling was characterized by X-ray diffraction (XRD) under controlled relative humidity (10–95% RH), while macroscopic swelling and water sorption were measured using dynamic vapor sorption (DVS). XRD analyses revealed that DC8- and DC10-treated samples exhibit a significant reduction in basal spacing variations, indicating efficient inhibition of interlayer swelling. DVS measurements confirmed lower water uptake and enhanced macroscopic dimensional stability of the clay pastes. Complete suppression of swelling was achieved at DC8 and DC10 loadings corresponding to only $\sim$35% of the CEC, suggesting strong interactions between protonated amines and clay layers. In contrast, diamines with longer chains, such as DC12, were less effective, indicating the existence of an optimal molecular length for inhibition. Overall, these findings demonstrate that partial cation exchange with alkyl diamines effectively stabilizes montmorillonite against swelling, providing a promising molecular-level strategy for developing durable and sustainable earthen construction materials.

Phase Diagram and Thermoelastic Properties of Iron Alloys at Telluric Planetary Core Conditions

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Poster 60

Keywords: iron alloys; phase diagram; thermoelastic properties; planetary cores; high-pressure experiments

Space missions combined with Earth-based observations are providing unprecedented geophysical data about the interiors of the telluric planets in the solar system. The InSight mission to Mars has delivered the first seismic records and improved geodetic measurements, enabling a better understanding of the red planet's interior. Meanwhile, BepiColombo is on its way to Mercury, and upcoming magnetic and gravity data will offer advances in deciphering the characteristics of this exotic planet. However, interpreting and fully exploitation geophysical data to build accurate models of planetary structure and dynamics—including internal convection and magnetic field generation—is still hampered by a lack of knowledge of the relevant material properties under the appropriate pressure and temperature conditions. All telluric planets share a basic layered structure: a central metallic core, primarily composed of iron, surrounded by a rocky mantle and a chemically differentiated crust. However, the elemental composition alloyed to iron in the core varies with the planet's distance from the Sun and the redox conditions prevailing during planetary formation and differentiation. Mercury, the most reduced telluric planet, likely contains significant amounts of silicon alloyed with sulfur in its core. Therefore, the Fe-S-Si system serves as the reference for modeling Mercury's core. In contrast, Mars, the outermost telluric planet, formed under more oxidizing conditions that prevent silicon incorporation into the core, which is instead expected to be enriched with oxygen and sulfur. Thus, the Fe-S-O system is used as an approximation for Mars's core. This PhD project aims to combine synchrotron measurements with high-pressure and high temperature experiments, along with electron microscopy of recovered samples, to investigate the Fe-S-Si and Fe-S-O systems. Determining phase diagrams and thermoelastic properties of stable solid phases will create the database needed to model the cores of mid-sized telluric planets, focusing on Mercury and Mars.

Fundamental Understanding and Stabilization Strategies of the Halide-Electrolyte/Anode Interface in All-Solid Halide Lithium Batteries

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Poster 40

Keywords: all-solid-state lithium metal batteries; halide solid electrolyte; $Li_3YBr_2Cl_4$ (LYBC); β-Li_3N; mixed-conducting interphase (MCI); lithium metal anode; lithium penetration; nano-holotomography; magnetron sputtering

All-solid-state lithium-metal batteries (ASSLBs) promise higher energy density and improved safety over conventional Li-ion cells. Among solid electrolytes, halide electrolytes such as $Li_3YBr_2Cl_4$ (LYBC) combine high room-temperature ionic conductivity with wide oxidative stability. Their main limitation is chemical instability against Li metal, which forms a mixed-conducting interphase (MCI) and leads to electrochemical failure. As a performance benchmark, we stabilized LYBC|Li with a sulfide interlayer (Li_6PS_5Cl), achieving low polarization and long life; however, the sulfide route is impractical due to H_2S risk, motivating an inorganic, halide-compatible alternative.

This thesis evaluates β-Li_3N as a protective interlayer. Compatibility tests confirm the (electro)chemical stability of β-Li_3N with LYBC and with Li. Full-cell cycling with 1–1.5 mm β-Li_3N layers reduces early overpotential, yet failure still develops with aging. Porosity measurements show β-$Li_3N \approx 32$ vol%, predisposing the nitride to Li penetration under stack pressure and during electrodeposition. Li–In anode full cells and unidirectional Li plating support this mechanism, which is directly visualized by synchrotron nano-holotomography, consistent with the emergence of an MCI and the observed polarization. We propose a degradation scenario in which Li infiltration short-circuits the Li^+ transport pathway in the β-Li_3N interlayer; subsequently, a substantial MCI forms at the LYBC|β-Li_3N interface, imposing high Li^+ resistance during discharge and ultimately causing halide-electrolyte degradation and capacity collapse.

Although β-Li_3N is chemically compatible, microstructure is the key factor: durable operation requires interlayers that are mechanically dense and crack-resistant. In the final phase of this thesis, we develop magnetron-sputtered nitride coatings and characterize them by GIXRD, SEM, and ToF-SIMS. By empirically optimizing target, Ar/N_2 ratio, power, and film thickness, we aim to produce electrochemically and mechanically robust coatings. Overall, this work provides processing guidelines for durable, halide-based ASSLBs and paves the way for scalable

manufacturing.

MOF/C composites for CO_2 capture by Microwave Swing Adsorption (MSA)

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Poster 63

Keywords: MOFs ; CO_2 capture ; Adsorption ; Regeneration ; Conductivity

The utilization of fossil fuels has grown rapidly, making them the main source of CO_2 emissions responsible for global warming. Emissions from fossil fuel combustion have more than doubled since the 1970s, now exceeding 32 Gt CO_2 per year. To mitigate climate change, carbon capture is essential to reduce atmospheric CO_2 release. Conventional capture technologies, such as amine-based solvents, face challenges due to high energy requirements and environmental impacts. In contrast, metal–organic frameworks (MOFs) have emerged as promising solid sorbents owing to their high CO_2 uptake and low regeneration energy. Notably, Calgary Framework 20 (CALF-20) was successfully scaled up by Svante and BASF in 2021 for post-combustion CO_2 capture.

As part of the National PEPR SPLEEN (CATALPA project), this work focuses on developing MOF/carbon composites to minimize desorption energy through microwave swing adsorption (MSA). Since pristine MOFs exhibit low electrical conductivity and poor microwave absorption, incorporating conductive carbon materials significantly enhances their microwave response. Previous studies demonstrated that MIL-91/graphene oxide (GO) composites achieved faster CO_2 desorption under MSA compared to conventional heating.

Here, MOFs such as CALF-20(Zn)[2], MIL-160(Al)[3], and MIL-120(Al)[4] were selected for their CO_2 selectivity, water stability, and scalable synthesis. A series of MOF/C composites were synthesized via in-situ and post-synthetic routes using varying carbon loadings. Remarkably, even 2 wt% carbon induced semi-conductive behavior in the composites. These conductive materials are now being evaluated for MSA regeneration in collaboration with Prof. Guy (Mons, Belgium). This presentation will highlight the synthesis, structural characterization, gas sorption properties, conductivity evaluation, and preliminary MSA regeneration performance of these novel MOF/C composites.

Orange Carotenoid Protein: Coupling Spectroscopic Measurements and Molecular Simulations

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Poster 33

Keywords: OCP ; photo ; activation ; carotenoids ; vibrational spectroscopy ; classical molecular dynamics ; time ; resolved spectroscopy ; solid matrices ; IR ; UV ; vis ; Resonance Raman

Orange Carotenoid Protein (OCP) is a two-domain carotenoprotein found as a photo-protecting agent in cyanobacteria. The photoprotective mechanism of OCP is based on photo-induced protein structural rearrangement during which the stable orange form turns into an activated red form that binds to specific light harvesting complexes and help dissipation of excess energy under strong illumination conditions. The relative structural simplicity and water-solubility make OCP a peculiar light-sensitive system in several fields, ranging from sensors to optogenetics.
The mechanism of forementioned is still under debate. This thesis has two objectives: investigation of carotenoid role in (photo-)activation, by vibrational spectroscopy and molecular dynamics; and establishment a chemically procedure to fabricate OCP.
Using classical MD is was found that in canthaxanthin-binding OCP (OCP-CAN) water molecules are located inside the N-terminal domain. More in details, a "water bridge" connects CAN to the NTD via hydrogen bonds, while other types of OCP do not show this behavior. This may explain the observed of a dehydration-induced activation of OCP-CAN observed experimentally.
Concerning photo-induced activation, time-resolved single flash IR spectra of OCP-CAN and OCP-ECN (echinenone-binding OCP) recorded on a dispersive IR spectrometer using synchrotron radiation has shown the presence of an early time intermediate, which was further investigated by time-resolved IR and Resonance Raman under continuous illumination.
Usually OCP is produced by expression of OCP in E. coli. This protocol allows only easy production of OCP-CAN or OCP-ECN; insertion of other carotenoids in the apoprotein is not possible. We explored "synthetic" procedure to build OCP from apo-OCP and isolated carotenoids. These

two building blocks were inserted sequentially in three matrices: Mesoporous Siliceous Foam, Metal Organic Frameworks and in Liposomes. Using UV-vis spectroscopy the presence of assembled OCP was observed. Further steps are under investigation in order to extract synthetic OCP from the matrices.

Towards new solid Mg^{2+} conducting electrolytes for post Lithium battery applications

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Poster 43

Keywords: Sulfide synthesis ; Energy storage ; Magnesium rechargeable batteries

Multivalent-based batteries, such as magnesium ion batteries could prove to be a promising complementary solution to current lithium and sodium ion technology. This relies on the ability to develop room-temperature ionic conductors for Mg^{2+}. As discussed in a theoretical study by Canepa et al. 2017 using DFT[1], high Mg^{2+} mobility could be reached if Mg^{2+} is located in an unfavorable coordination environment, i.e. different than 6. With Mg^{2+} occupying tetrahedral sites, cubic direct spinel structure MgB_2X_4 perfectly meets this requirement. Indeed, $MgSc_2Se_4$ experimentally shows good RT-ionic conductivity. Unfortunately, selenium and scandium are, respectively, toxic and an expensive rare earth. Therefore, $MgAl_2S_4$ is proposed as an interesting alternative.

This composition does not crystallize in the Fd-3m space group (cubic spinel) using conventional solid-state synthesis, usually favoring either R-3m or Pnma space groups. Although presumably, magnesium is 6-fold coordinated in these structures, understanding the stability of these two polymorphs, isolating them and measuring their properties remains interesting and challenging. Using another synthesis route, inspired by a study done by Duan et al. 2022[2], we successfully stabilized the spinel system via high-pressure high-temperature synthesis technique. Although XRD refinement confirms a chalcospinel phase, determining the inversion coefficient remains tricky. ^{27}Al solid-state NMR measurements prove essential in determining the aluminium coordination environment and deducing that of the magnesium. The synthesis method remains to be optimized and further studied. Conductivity will be probed using temperature-dependent electrochemical impedance spectroscopy when sufficiently pure samples are obtained.

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Tuning the coalescence rate over orders of magnitude in liquid mixtures of simple surface rheology

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Poster 20

Keywords: bubbles ; coalescence ; interfaces

Bubbles and foams formed in oil mixtures exhibit lifetimes that are orders of magnitude longer than those formed in pure liquids even though they are surfactant-free. A previous work in our team1 has shown that foam stability is ensured by a surfactant-like effect of the molecules with the lowest surface tension in the mixture. In the thin liquid film created between two bubbles, this translates into an effect analogous to Gibbs elasticity - surface tension decreasing as thickness increases - which is low, but sufficient to ensure the film's relative resistance to stretching and hence to thinning. Hence, in these systems, a thermodynamic effect sets the boundary conditions at the film interfaces with air and combines with the flows to determine the film lifetimes. In addition, the behavior of the films interface finely depends on the mixture composition. In order to obtain quantitative descriptions of the couplings between the bulk (drainage) and interfacial transfers, we offer to systematically investigate the effect of the bubbles curvature on their lifetime.

To do so, we have developed a millifluidic experimental set-up to measure the lifetime of liquid films between two bubbles flowing in tubes of varied diameter D so that we control the bubbles curvature. We use a series of binary oil mixtures composed of decane and cyclopentanol in varying proportions so that we vary the interface elasticity mentioned above. Bubble trains are generated by injecting nitrogen into a cylindrical tube, through which the oil mixture circulates, controlling the liquid flow rate and the gas pressure.

Bio-based polymers for the development of innovative waterborne latexes

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Poster 50

Keywords: Bio ; based ; RAFT ; PISA ; Self ; assembly

The growing global environmental issues and the depletion of fossil fuel resources have increased the interest in developing sustainable bio-based polymers. Bio-based monomers are mainly obtained from 4 groups of renewable resources : terpenes, carbohydrates, lipids and lignin. Many studies have described the radical polymerization of monomers derived from the latter, leading to the formation of polymer that are usually fully hydrophobic [1]. There are then few examples of amphiphilic bio-based block copolymer in the literature [2,3]. In this work, we propose the synthesis of amphiphilic diblock copolymers via the environmentally friendly RAFT-PISA [4] process in water. In a series of experiments, a hydrophilic macroRAFT agent was extended in water with a hydrophobic bio-based monomer. The extensions of the first block were controlled, as evidenced by size-exclusion chromatography (SEC) and led to the formation of nanoparticles. The effect of parameters such as the concentration and the length of the hydrophobic block on the morphologies and on the particle sizes was then studied by dynamic light scattering (DLS) and cryogenic transmission electron-microscopy (cryo-TEM).

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Description of reaction intermediates by time-resolved solid-state NMR

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Poster 17

Keywords: calcium carbonate ; solid ; state NMR ; inorganic chemistry

Calcium carbonate ($CaCO_3$) is a mineral of major importance in Biology and Earth Science as it is involved in biomineralization processes [1]. Recent studies have shown that $CaCO_3$ tends to not follow the classical nucleation theory. In opposition to this one step process, recent studies have shown that $CaCO_3$ crystallization follows a non-classical nucleation pathway involving various soluble and solid intermediates [2]. These transient phases are particularly challenging to characterize as 1) they can exhibit very short life-times (below seconds) [3] and 2) isolation or drying methods can have deleterious and irreversible modification of their structures.
In order to study these transient intermediates in their native environment, we are currently developing an original approach consisting in sample cryo-fixation combined to low-temperature solid-state NMR analysis [4]. First, mineralizing $CaCO_3$ solutions are prepared with a stopped-flow device, allowing to reach very short reaction times (∼10 ms). Then, the resulting solution is transferred to a freeze-quench accessory where it is vitrified into cold isopentane (∼-140∘C). Finally, the cryo-fixed samples are transferred into the cold NMR probe (-120∘C). Transient intermediates are thus stabilized and preserved during the solid-state NMR analysis.
As the carbonate speciation (HCO_3-vsCO_3^{2-} is a key parameter of PNC or ACC structure, we first analyzed cryofixed NaHCO3 solutions through low-temperature ^{13}C solid-state NMR at various pH and concentrations. Finally, analysis of $CaCO_3$ mineralizing solution at short reaction time (10 ms to few sec.) will be shown demonstrating the possibility to investigate short-lived CaCO3 transient intermediates through time-resolved solid-state NMR.

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How to colour glass in green

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Poster 13

Keywords: green glass ; OAS ; glassmaking history ; colour ; stained ; glass

One of the major challenges of stained-glass windows restoration lies in the choice of filling glass pieces that will agree with the original artwork. The evolution of glassmaking traditions over time lead to changes in the accessible colour palette. The history of green colouring is a telling example of this evolution. Since ancient Rome, green colouring, although absent from a large number of arts and crafts, has been widespread in glassmaking [1], where iron impurities give a naturally greenish tint to glassy objects. By using copper, in addition to iron and in different proportions, the accessible green palette is extended and nuanced [2, 3, 4]. The use of green spread during the central Middle Ages [1, 2], accompanying major changes in glass compositions. Iron and copper, however, remained the only green chromophores used to colour the stained-glass windows. Nowadays, the range of green shades available to glass artists is wider, thanks to the use of new chromophores such as chromium [4, 5].

In this study, we established a chronology of the green chromophores used to color stained glass from the 12th century to the present day. To this extent, we studied a corpus of historical glass pieces with optical absorption spectroscopy (OAS). Combined with the chemical composition of the pieces, these results enable to compare the glass production conditions and therefore the evolution of glassmaking craftsmanship through time.

The study of a large number of contemporary pieces made it possible to highlight a joint use of several chromophores to produce green colorations, enriching the accessible palette and making the link between colour and composition more tenuous.

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Design of advanced carbide nanocatalysts for substitution of noble metals in heterogeneous catalysis

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Poster 6

Keywords: Catalysis ; transition metal carbides ; in situ characterisation ; X-ray absorption spectroscopy

Transition metal carbides (TMCs) based on molybdenum and tungsten are promising substitutes for noble metals in selective hydrogenation due to their tunable electronic structure and high resistance to deactivation. This work explores how different preparation routes and compositions govern the structural evolution and catalytic behavior of Mo/W bicarbides supported on carbon and zirconia. A series of mono- and bimetallic catalysts (MoC, WC, Mo_3W_1/C) were synthesized via co-impregnation or sequential two-step carburization under CH_4/H_2, and characterized by XRD, TEM, and BET analysis. Operando X-ray absorption spectroscopy (Mo K- and W L_3-edges) combined with multivariate curve resolution–alternating least squares (MCR-ALS) decomposition was employed to resolve the speciation dynamics during temperature-programmed carburization. The analysis revealed distinct kinetic pathways depending on the synthesis sequence: the Mo-first route promoted an early carbide formation through Mo-assisted W reduction, whereas the W-first route favored a delayed, oxide-driven carburization. The onset and persistence of oxide, reduced-oxide, and carbide components ("dominance windows") were directly correlated to the resulting microstructure and catalytic response.

Catalytic tests in the selective hydrogenation of acetylene to ethylene demonstrated that bimetallic carbides outperform their monometallic counterparts in both activity and selectivity. The optimized Mo_3W_1/C sample exhibited stable conversion with suppressed over-hydrogenation, reflecting a balanced surface composition of Mo- and W-carbide domains that tune hydrogen activation and C_2H_2 adsorption energetics.

Overall, this study establishes a direct link between in situ XAS-derived speciation and catalytic performance, highlighting the importance of controlling oxide-to-carbide transformation pathways in the rational design of noble-metal-free hydrogenation catalysts.

Infrared hyperspectral imaging system, low noise and its extension to integral field infrared spectroscopy

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Poster 46

Keywords: hyperspectral imaging ; short wave infrared (SWIR) ; optoelectronics ; interferometry ; data processing and reduction ; field programmable gate array (FPGA)

Since several decades, imaging has become ubiquitous and a strategic tool in fields such as industry, medicine, military and science.
Firstly limited to the visible spectrum, the wavelengths detections requirements have quickly evolved to ultraviolet and infrared bands. In this last band, detections in the SWIR (Short Wave Infra Red) are essentials. Indeed, they are exploitable with few limitations related to the black body at ambient temperature, which can permit detection with very low photon flux. SWIR detections are also providing a very wide of field of interests and applications such as materials research and characterization (for instance new materials such as Graphene, quantum boxes, nanotubes), interactions (between a characterized material and human tissues for instance), biological applications, biomedicine, telecommunications laser sources, military applications, industry uses (real time and non-destructive quality control in fabrication processes), etc.
A significant number of these use cases, if not all of them, require access to increasingly sophisticated infrared detection systems, Thus, more sensibility and less readout noise and as a result, more SNR (signal-to-noise ratio) are always needed. Video dynamic range, resolution and framerate must be highers as possible. Furthermore, in addition to the above-mentioned constraints, the need of performing multispectral or sometimes hyperspectral acquisitions has become a must. High wavelengths selectivity is also become a key to perform some measurements such as dissociate materials or increasing the contrast of signals to be studied.
In this project, all of these requirements will be combined to design and develop a low noise infrared hyperspectral imaging system with prospects to full-field infrared spectrography. Beyond the technical solutions to be found and implemented, a major focus will be given on the data hypercube processing and reduction by considering innovative methods.

MoS_2/MIL-120 composites for CO_2 absorption and directly photocatalytic reduction

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Poster 78

Keywords: Metal organic frameworks ; composites ; CO_2 adsorption ; photocatalytic CO_2 reduction

From an economic and environmental point of view, photocatalytic CO_2 conversion into value-added chemical feedstocks is one of the most promising techniques to mitigate environmental issues and the energy crisis. In this regard, Metal-organic frameworks (MOFs), due to their specific crystalline structures, tailorable pore environments, and extensive structural diversity, have emerged as promising platforms for specific properties such as visible light response and high CO_2 adsorption capacities, as well as the possibility to construct heterojunctions with various entities, among others. For instance, MIL-120(Al) with pores being decorated with a high density of μ_2-OH groups as well as accessible aromatic rings, have demonstrated exceptional CO_2 uptake, and stand as one of the benchmarks in this domain. However, the vast majority of bare MOFs with high CO_2 uptakes are poorly or not photo(catalytically)active. On the other side, pure semiconductors materials, such as MoS_2, TiO_2 and Co_3O_4, possess high redox capabilities but suffer from the swift photo-charge recombination and poor affinity for CO_2, which significantly limits their photocatalytic activity and results in the low product selectivity. Thus, designing excellent MOF-Semiconductor (MOF-SC) composites photocatalyst with exceptional CO_2 uptake and high photocatalytic CO_2 reduction activity is very appealing and promising. Thus, I have explored different MOFs and semiconductors for finding optimal MOF-SC composites. In this presentation, I will focus on MoS_2/MIL-120(Al) composites, constructed from MoS_2 for its good photosensitivity and catalytic activity,together with the MIL-120(Al) to promote higher CO_2 concentration near by the active sites. This will promote photocatalytic CO_2 reduction thanks to the photogenerated electrons. Besides, I will also discuss the benefit of electrostatically co-assembling of MOF-SC composites with TiO_2 and Co_3O_4 to avoid the usage of sacrificial agents and to capture photogenerated holes for photocatalytic water oxidation, when irradiated with 300 W Xenon lamps in solid-gas (CO_2 gas and water vapor) system.

Perfusion of macroporous collagen hydrogels generated by 3D printing and cellularized to model the healthy and fibrotic skeletal muscle

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Poster 74

Keywords: Collagen ; Hydrogel ; 3D printing ; Muscle ; Perfusion ; Fibrosis ; OCT ; In vitro model

Duchenne Muscular Dystrophy (DMD) is a genetic disease causing muscle degeneration due to absence of dystrophin. Consequently, the muscle extracellular matrix (ECM) becomes fibrotic, with excessive type I collagen replacing functional muscle tissue, leading to increased stiffness, reduced nutrient and oxygen perfusion, and impaired muscle contraction. Existing DMD models remain inadequate, as 2D cell cultures lack 3D structure and cell-ECM interactions, and animal models present species differences. To overcome these limitations, we developed a 3D printed collagen-based muscle ECM reproducing both healthy and fibrotic environments, integrated into a microfluidic chip. A multi-layered pattern was used, with intrinsic porosity controlled by adjusting the number of collagen filaments per layer. Porosity was quantified using Optical Coherence Tomography (OCT). Increasing layer density reduced porosity from 6% to 2%, doubling perfusion time from ∼6 min to >20 min, thus mimicking fibrotic muscle perfusion. Stiffness was increased by collagen chemical crosslinking using EDC/NHS reagents. Mechanical properties were increased from ∼20 kPa to ∼100 kPa, as evidenced by tensile testing, replicating the final stage of fibrosis. Tensile testing also showed that porosity did not significantly influence Young's modulus, confirming that this parameter could be modulated independently of stiffness. The impact of reduced porosity was then evaluated after 3D cellularization into two 600 μm-diameter channels, combining immunofluorescence to observe cell morphology and dynamic OCT that provides label-free imaging of cell metabolism. Low porosity decreased C2C12 myoblast metabolic activity (from 0.6-5 Hz to –0.3 Hz range), while cell morphology remained similar in both healthy and fibrotic conditions. These results highlight the significant impact of reduced perfusion on cell metabolism in 3D muscle ECM. This model accurately replicates the decreased porosity and stiffness of fibrotic muscle ECM, providing a tunable platform to study the impact of fibrosis.

Effect of enhanced foaming capacities of binary liquid mixtures on vertical two-phase flow regimes

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Poster 32

Keywords: Gas ; liquid flow ; Foaming liquids ; Binary mixture

This study focuses on the regimes of gas-liquid vertical flows in stagnant liquids displaying foaming properties. The liquids investigated are binary mixtures of miscible oils, which exhibits foaming properties without any surfactant. These foaming properties have recently been studied in our laboratories1 and ascribed to an enhanced stability of the thin liquid films separating bubbles. The present study aims at highlighting the effect of those foaming abilities on the vertical two-phase flow regimes, usually studied on non-foaming pure liquids or aqueous solutions. The gas-liquid flows are generated by injecting nitrogen through a sinter at the bottom of a glass column, in an original setup derived from the classical Bikerman method2, commonly used for measuring the foamability of liquids.

In the first place, gas-liquid flows with pure, non-foaming liquids are investigated through several parameters, namely the initial liquid height inserted, the generated bubble sizes, and the column's diameter. Secondly, the effect of the liquid's foamability on the flow regimes is investigated, the adjustment of the molar fractions of each components allowing us to tune the foaming properties of the system on a wide range. In our first experiments on foaming gas-liquid flows, we observed that the addition of small molar fractions of the second miscible liquid in the binary mixture leads to new flow regimes in which large gas pockets coexist with liquid slugs with numerous small bubbles. In practical applications, where liquids are often mixtures, we believe that our results will have important implications, notably in predicting the gas-liquid flow regimes.

MOF-Based Microneedles for Synergistic NO/ · OH Antibacterial Therapy

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Poster 72

Keywords: Metal organic frameworks ; Microneedles ; Nitric oxide gas therapy ; ferroptosis

Bacterial infections pose a significant threat to global health, exacerbated by the rise of drug-resistant bacteria due to the misuse of antibiotics.[1] Recently, gaseous nitric oxide (NO) has attracted enormous attention in antibacterial applications.[2] L-arginine (L-arg), a biocompatible amino acid, reacts with excessive hydrogen peroxide (H2O2) in wounds to release NO via a non-enzymatic pathway, ensuring high biosafety.[3] However, direct L-arg delivery faces challenges like short half-life and low bioavailability, necessitating efficient delivery systems. Metal-organic frameworks (MOFs) are porous crystalline materials composed of metal ions and organic ligands. The structural diversity and tunable pore sizes of MOFs make them ideal carriers for therapeutic agents. Among them, MIL-100(Fe) (MIL stands for Materials Institute Lavoisier), a benchmark mesoporous iron trimesate MOF nanocarrier, stands out for good biocompatibility, high drug-loading capacity, and biodegradability.[4] Moreover, MIL-100(Fe) is promising for the Fenton reaction to produce hydroxyl radicals (· OH) and induce ferroptosis-like bacteria death.[5] Additionally, MIL-100(Fe) excellent chemical stability allows this nanoMOF to be processed into diverse formats,[4] significantly expanding its utility in medical devices. In our study, L-arg was encapsulated into MIL-100(Fe) particles through physical adsorption. MIL-100(Fe)@L-arg, along with lactate oxidase (LOx), which catalyzes the conversion of excess lactate in wound area into H2O2, was incorporated into a polymer matrix to fabricate microneedle patches using 3D-printed molds. When applied to wounds, the patches dissolved in the wound environment, releasing LOx and MIL-100(Fe)@L-arg particles. In the presence of H2O2, the synergistic production of NO and · OH worked to effectively kill bacteria and promote wound healing.

Study of the relation between structure and composition of biobased dimer acids monomers and chemical structure and properties of resulting polyesters

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Poster 66

Keywords: Biobased ; Characterization ; Dimer Acids ; Polyesters

Polyesters resins synthesized from biobased dimer acids monomers are used in many different applications, such as coatings, inks, adhesives, lubricants [1]. Dimer acids are composed mostly of dicarboxylic acids (diacids), but some monoacids and triacids are present [2]. The mixture of these compounds corresponds to dimer acids. The mechanism of formation of dimer acids is still often assumed to be through a Diels-Alder mechanism although experimental evidences only support an electrophilic addition mechanism [3]. Literature shows only a few different structures to illustrate this mechanism but the structure elucidation is far from complete. The chemical structure of the dimer acid has an impact on the properties of the resulting polymer, such as chemical stability [4]. Composition of dimer acid sample will influence polymerization process: monoacids tend to stop the polymerization, while diacids will add elongation and triacids some branching. Knowing that, the first objective is to characterize dimer acids samples by determinizing their composition and molecular structures.

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Experimental and theoretical investigation of X-ray optical activity in paramagnetic chiral system

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Poster 22

Keywords: Chirality ; optical activity ; electronic properties

Chirality refers to a crystal that lacks certain symmetry operations (for example mirror planes) and is often linked to optical activity — the different interaction of a material with left- and right-handed circularly polarized light. While optical activity is well studied in the ultraviolet–visible range, it has been much less explored at X-ray energies. This work investigates three X-ray effects in a single chiral compound: X-ray magnetic circular dichroism (XMCD), X-ray natural circular dichroism (XNCD), and X-ray magnetochiral dichroism (XMχD). We focus on X-ray absorption near-edge spectroscopy (XANES) at the cobalt K-edge for the metal–organic complex $[Co(en)_3](NO_3)_2$, which crystallizes in space group P6322 — a symmetry that is compatible with XNCD [1]. The compound is a single, uniaxial chiral crystal containing high-spin Co(II). We combined experimental measurements and theoretical calculations to study how the compound responds to different X-ray polarizations. Experimentally, spectra were collected at the ID12 beamline of the ESRF (Grenoble), which provides precise control of X-ray polarization. Theoretically, calculations were performed within Density Functional Theory (DFT) using the FDMNES code. A full-potential, finite-difference method — going beyond the usual spherical "muffin-tin" approximation — was employed to compute the excited states [2]. The main result is clear: the good agreement between experiment and theory shows that XNCD can be an effective probe of chirality in certain compounds, and that modern theoretical approaches can robustly support the interpretation of experimental data. In addition, a theoretical study of optical active compounds will be devoted to provide a solid background for the interpretation of experimental spectra in this research.

Understanding defects in nanomaterials by multiscale structural analysis: Boron Phosphide case study

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Poster 26

Keywords: PDF analysis ; Boron phosphide ; nanomaterials ; defects

Nanomaterials often possess new/enhanced properties compared to same macro/micromaterials, mainly due to their important surface to bulk ratio[1]. At their surface, atoms cannot complete their coordination sphere, therefore a plethora of defects in various forms appear. Due to size constriction and proportion of defects, many techniques of characterization fail to identify correctly the structure of nanomaterials. We propose in this PhD to detect, identify and describe local defects in nanomaterials by Pair Distribution Function (PDF) analysis. This G(r) function, shows all atomic pairs separated by a distance r in a material[2]. Calculation from a model compared to experimental PDF curves, allows to understand and describe long range as well as short-range organization in material, including nanoparticles and amorphous material. The final objective is to have a firm methodology to tackle each types of defects encountered, for any materials.

Many systems where analyzed in collaboration with researchers at the LCMCP: AlOOH to Al_2O_3, Ag_2S, $WO_3.H_2O$, molten salts LiI-KI... We will focus here on boron phosphide BP, interesting materials for photo(electro)catalysis, hardness or for its semi-conductor properties[3,4]. Nanomaterial BP synthesized in molten salts was analyzed first by ex-situ PDF analysis, then during in-situ annealing and in situ synthesis in molten salts. Additionally, in situ annealing in high pressure and temperature was followed by diffraction. The results of those experiments tend to show the presence of two kind of defects, at the surface and in the nanoparticle core and allow us to discuss synthesis mechanism.

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New synthesis of polymeric Janus nanorods

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Poster 71

Keywords: Janus nanoparticles ; controlled radical polymerizaiton ; RAFT ; ATRP ; self ; assembly

We recently developed an original method to prepare Janus nanorods that allows us to obtain cylindric nanoparticles in which the faces are constituted of different polymers [1]. The elaboration of the Janus nanorods is based on the use of a supramolecular sticker that induces the assembly into cylinders. These nanoparticles have potential applications in different fields such as nanomedicine, nanolithography and catalysis [2]. Our objective is to improve the synthesis methodology of these nanoparticles, especially to reach higher molar masses. During my PhD, a tris-urea based transfer agent and initiator have been synthesized. They have been used to perform RAFT [3] (Radical Addition-Fragmentation Transfert) polymerization and ATRP [4] (Atom Transfert Radical Polymerization) of various monomers. The corresponding polymers have been characterized by NMR (^{13}H and ^{13}C), SEC, MALDI. The synthesized polymers have been used to form Janus nanorods by a co-solvent procedure. The nanoparticles obtained have been characterized by electron microscopy and SAXS.

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Study of biomimetic membranes composed of glycosylated lipids

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Poster 68

Keywords: Biosurfactants ; lipids ; cosmetics ; depollution ; drug delivery ; vesicles ; supramolecular chemistry ; nanochemistry

Bio-based surfactants, derived from biomass via fermentation of glucose and vegetable oils, have gained popularity due to their eco-friendly advantage over petroleum-derived surfactants, which rely on the pollutive chemical processes. Microbial glycolipids (MGs) are bio-based surfactants, and their amphiphilic nature enables them to interact with lipid bilayer membranes, a key structure in all living organisms, while also exhibiting antibacterial, anticancer, and antiviral properties. Modification to lipid membranes can significantly impact cell function, highlighting the potential of MGs in diverse applications. The self-assembly of microbial (MGs) into bilayers and their impact on biological membranes remains underexplored. Some key biophysical properties are not well understood. This study is focused on exploring the biophysical properties of membrane-forming MGs and their interaction with phospholipid-based biomimetic membranes. Biosurfactants known to form membrane-like structures, such as Acetylated G-C18:1, Acetylated Lactonic SL-C18:1, mono-rhamnolipid,and trehalolipids, were prepared. Lamellar structures were prepared using Milli-Q water (18.2 MW). The pH is adjusted using NaOH and HCl solutions (0.5M, 1M, and 5M). Fibrillation was induced with calcium chloride ($CaCl_2$) as a source of Ca^{2+} ions. The glycolipids studied included Glucolipids (G-C18:1, G-C18:0) and Sophorolipids (SL-C18:1, SL-C18:0). Phospholipid vesicles, including DOPC (1,2-Dioleoyl-sn-glycero-3-phosphocholine) and DPPC (1,2-Dipalmitoylphosphatidylcholine), were synthesized in uni-lamellar vesicles (ULVs) and multi-lamellar vesicles (MLVs) forms to study the amphiphilic interactions.

Biophysical properties of membrane-forming biosurfactants were analyzed using small-angle X-ray scattering (SAXS), small-angle neutron scattering (SANS), neutron spin-echo (NSE), differential scanning calorimetry (DSC), and Langmuir-Blodgett Trough, revealing bilayer thickness, bending rigidity, melting temperature, and area/molecule. Similar techniques are aimed to be used further to elaborate on MGs and PLs.

The results align with the project objectives. Further refinement of SAXS and SANS data is ongoing. Confocal microscopy is needed to confirm Giant unilamellar Vesicle (GUV) formation and glycolipid effects, with GUV protocols requiring optimization through several trails.