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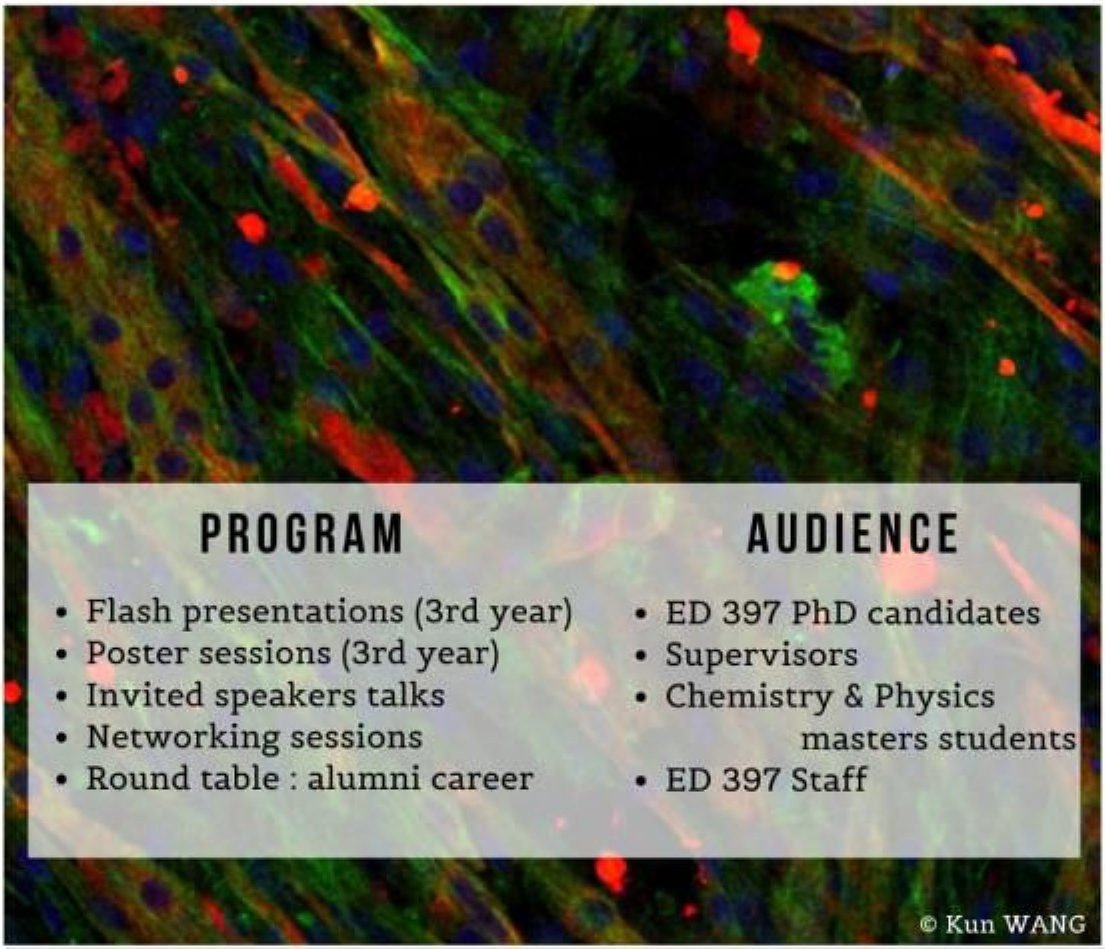

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High performance layered oxide synthesis based on Ni, Mn and Co : development of an industrial process and application to the positive electrode of a Li-ion accumulator

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Abstract

The objective of this thesis work is to synthesize materials based on nickel, manganese and cobalt (NMC) leading to compositions enriched in nickel (Ni-rich) or over-lithiated (Li-rich) using an alternative synthetic method to the traditional coprecipitation method.
Indeed, the gigafactorie advent implies ever increasing production costs of materials and batteries in order to obtain the necessary economies of scale for their economic profitability. Thanks to the ceramic-process know-how of the company Nanoe in collaboration with the Laboratory of Chimie de la Matière Condensée de Paris (LCMCP), an industrial solid synthesis process has been developed for the production of positive electrode materials.
The new process developed should allow a more economical synthesis (atom economy, shorter process, lower energy expenditure, less expensive precursors) without rejecting solution waste as the coprecipitation process.

Keywords: Material science, Electrochemistry, Li, ion accumulator, Layered oxide, industrial process

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Synthesis and characterization of MOF based selective membranes for Lithium–Sulfur Batteries

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Abstract

Lithium-sulfur batteries display high theoretical specific capacity (1675 mA h g-1) and are among the most promising solutions for sustainable energy storage systems with high energy density (2600 W h kg-1). However, during the charging/discharging process, the redox intermediates polysulfides (Li2Sx, $3 \leq n \leq 8$) easily migrate through the traditional separator and interact with lithium anode, causing the anode' passivation with a layer of insoluble and non-conductive Li2S/Li2S2, which leads to a loss of active material and a low cycling stability of the battery.[1] To overcome these limitations, functional materials with enhanced selectivity towards polysulfides species have been developed.[2-3] Metal-Organic Frameworks (MOFs) appear as strong candidates to limit polysulfides migration.[4] Built-up from metal ions or clusters coordinated to organic ligands, their crystalline porous network can be easily tuned (pore size/shape, hydrophilic character, Lewis/Bronsted acid...) to achieve a desired property.

We focus on the design of MOF based membranes as selective interlayers to mitigate the diffusion of polysulfides. A series of highly stable MOFs has been prepared and included in mixed matrix membranes. Different parameters, such as MOF/polymer pair, MOF particles size, MOF content and membrane thickness have been explored. Homogeneous membranes with good mechanical stability were obtained and have shown to successfully retain the diffusion of polysulfides.

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Keywords: Lithium, sulfur batteries, Metal, Organic Frameworks

Structural elucidation of nano-sized metal-organic frameworks using three-dimensional electron diffraction

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Abstract

Metal-organic frameworks (MOFs) are hybrid crystalline porous solids demonstrating potential applications in different domains related to energy, environment or health [1]. However, the synthesis of robust MOFs often leads to polycrystalline compounds rendering the structure elucidation by single-crystal and powder X-ray diffraction challenging. A good alternative is to solve the structure from 3-dimensional electron diffraction (3DED) data [2], a method allowing to solve the structure from much smaller volumes by using electrons instead of X-rays (Figure 1a). This project focuses on the structural elucidation of nano-sized MOFs providing a better understanding of their unique properties. In addition to diffraction-based techniques, other complementary structural characterization methods such as pair distribution function analysis and low-dose high-resolution TEM (LD-HRTEM) were used. Due to the high electron beam sensitivity of MOFs, the latter was only made possible by the use of a microscope equipped with a direct detection electron counting camera (DDEC) [3], enabling the imaging of MOFs with low dose rates. Titanium-based MOFs (Ti-MOFs) exhibit good chemical and thermal stability, high porosity and redox activity which makes them good candidates for applications such as photocatalysis [4,5]. We have synthesized a new robust nano-sized Ti-MOF named MIP-21X, yet its structure solution from the powder diffraction data has been found challenging due the presence of only few broad peaks. Two strategies were undertaken: the PDF analysis enabled the deduction of the arrangement of the titanium atoms constituting the clusters, then a predicted model has been proposed and subsequently validated using LD-HRTEM images of the MOF (Figure 1b), from which we could extract the unit cell parameters, the diameter of the channels and the arrangement of the Ti-oxo-clusters. As a second strategy, the structure has been successfully solved ab initio from 3DED data.

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Keywords: Metal organic frameworks, Low dose high resolution TEM, three dimentional electron diffraction, Structure determination

Interactions between Orange Carotenoid Protein and mesoporous silica: from fundamental research to the development of photoactivable nanodevices

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Abstract

The photoactive Orange Carotenoid Protein (OCP) is a protein involved in photo-protective responses in cyanobacteria. It induces the thermal dissipation of excess solar energy counteracting oxidative stress and photodamage. OCP consists of two structural domains sharing a non-covalently linked antioxidant carotenoid as a cofactor. Blue light induces photoactivation of OCP and its colour changes from orange to red. SBA-15 (Santa Barbara Amorphous) was chosen as an inorganic support for OCP. These materials have attracted much attention as hosts for immobilization of enzymes as well as delivery systems. The structural parameters of SBA-15, such as the diameter of pores and micro-porosity can be modified by tuning parameters of its synthesis. Besides to the possibility of adjusting the size of the pores, the ability to modify the surface properties of these materials to match the targeted biomolecules can provide higher protein immobilization capacity. In this work we have immobilized OCP on different kinds of raw and surface-functionalized SBA-15 mesoporous silica nanoparticles and structurally characterized the systems. SBA-15 matrices have demonstrated to be suitable supports for OCP, whose immobilization is strongly enhanced by the pre-photoactivation of the protein. OCP remains photoactive inside the mesoporous silica matrix, thereby producing photochromic nanoparticles. Under appropriate conditions OCP can also be released from SBA-15 nanoparticles. This work is a first step to understand the influence of matrix constraint on OCP photo-properties. Furthermore, this research demonstrates that the OCP@SBA-15 system can be used as a photochromic material and as a possible optical device for nanoscale applications, notably as optical sensor for pH or temperature and as photoactive switch for the development of tunable-emission silica fluorescent NPs for imaging. Finally, this work is a first step towards the development of caroteno-protein and carotenoid release-strategies from silica matrix to be applied in the field of antioxidant drug delivery.

Keywords: Orange Carotenoid Protein, mesoporous silica, drug delivery, nanodevices, FTIR spectroscopy, photochromic devices

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*Speaker

Biocompatible and stimuli responsive nanoMOFs for innovative biomedical applications

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Abstract

Introduction: Although MOFs possess amounts of features that make them attractive materials for a wide range of potential applications, increasing attention has been paid, in recent decades, to their use in biomedicine. So far, most studies have focused almost exclusively on their efficacy in killing pathogenic cells, once loaded with active drugs, but little has been done to assess their fate when administered to the body. One of the main reasons is related to the significant limitations still to be addressed, represented by a lack of control of the dispersion and/or stability of the particle size once in contact with body fluids.
The main target of this project is to achieve better control of the nanoMOF properties and size while keeping their crystallinity and porosity under physiological conditions.

Methods: bare or surface-functionalized nanoMOFs were prepared.[1] The first MOF candidate is MIL-100(Fe),[2] a mesoporous iron trimesate MOF that was synthesized as nanoparticles smaller than 100 nm. In order to obtain stable nanoparticles without aggregating in simulated body fluids, various conditions have been tried to establish the functionalization of MOFs external surface.
Results: Both the colloidal and chemical stability of the modified nanoMOFs particles have been improved compared with bare MOFs, with almost no change in crystallinity and porosity according to PXRD and BET analysis.

Keywords: Non, Pharmaceutical Agent, MOFs, Stability, Nanoparticles, Coating

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Density measurement of Fe-C-S alloys under Moon's core condition

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Abstract

Sulfur and carbon are considered as two dominant light elements incorporated with iron in the Moon's core. The physical properties of liquid Fe-C-S are thus crucial for understanding today's composition of the Moon's core, as well as the core evolution process since the formation of the Moon 4.5 billion years ago. In this work, the liquid structure and density of Fe-C-S alloys containing up to 1.5 wt%C and 30 wt%S have been studied *in situ* at high pressure and high temperature (1-5 GPa and up to 1900 K) by combined angle and energy dispersive X-ray diffraction (CAESAR) and X-ray absorption experiments performed

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[*] Speaker

in a Paris-Edinburgh press, and by electron microprobe analysis of the recovered samples. The local structure of liquid Fe-C-S alloys shows no obvious modification from that of iron, suggesting that the Moon's core with low light element content probably retains similar compressibility to pure iron. Density of the alloys has been extracted from the diffuse scattering by minimization of the oscillation in the short distance of the radial distribution function g(r). A thermodynamic model has been developed for the density of the ternary Fe-C-S system as a function of pressure, temperature, and light element content. Obtained dataset and derived model are used to address structure and composition of the core of the Moon.

Keywords: Density, iron alloys, high pressure, in situ, Moon core

Synthesis, characterization and development of new bio-sourced Low Molecular Weight Gelators (LMWGs)

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Abstract

Low molecular weight gelators (LMWGs) are organic compounds that are able to turn liquids into gels when they self-assemble into a fibrous network of anisotropic. Indeed, this type of molecules can be used in numerous applications, such as cosmetic, lubricant or tissues engineering. A very wide range of materials have been recognized since the 1860's to form gels, often with quite different characteristics. During the 1990s, several compounds were known to induce supramolecular gels like urea, amides, sugars, fatty acids, and many others. The point in common of these compounds is that the gelator characteristics have been discovered by serendipity. In fact, the phenomenon of gelation is quite difficult to predict and needs several studies of structure-property relationships. A primordial point is to be careful to the solubility of the LMWGs because, if it is too soluble in solution, it will have no possibility to form the strong intermolecular networks. Moreover, a lack of solubility will induce the precipitation of the LMWGs making it inefficient. This project has the aim of developing new bio-sourced low molecular weight gelators, using the most natural products or bio-sourced blocks possible while trying to respect the green chemistry principles.

Keywords: bio, sourced, gels, amides, assembly, characterization

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*Speaker

Synthesis of supramolecular polymers for the reinforcement of bitumen

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Abstract

Due to a steady increase of the traffic together with an increase in the speed and load of the vehicles, the roadways are more and more stressed. This has the consequence of reducing their service life while the maintenance costs are raising up. Moreover, roads in poor conditions (cracking, potholes, etc.) leads to an increase of the CO2 emissions from cars ranging from 5% to 9% depending on the condition of the road. Improving the properties of bitumen, an essential material with aggregates and sand in the production of roads, is therefore a current issue.
Several additives are developed in order to improve the properties of bitumen like its hardness, its resistance to rutting. Unfortunately, the addition of these molecules (mainly polymers) into bitumen is leading to an increase in viscosity and therefore to an increase in the processing temperatures. This implies harmful emissions that can affect the health of workers as well as higher energy costs.

The objective of my thesis is to develop an additive able to improve the mechanical performance of bitumen at service temperatures while limiting the increase in viscosity at processing temperatures to avoid the drawbacks presented before.
Thanks to their reversible nature, the use of organogelator seems to be an attractive approach. Indeed, the molecules will assemble via hydrogen bonds to form supramolecular strands which will subsequently self-assemble into fibers. It will allow the formation of a three-dimensional fibrillar network that will ensure the mechanical reinforcement of the bitumen at service temperatures. The particularity of this fibers' network is to be thermoreversible (the weak energy bonds established will be able to break under heating), which will avoid any increase in viscosity at processing temperatures.

Keywords: Supramolecular chemistry, Hydrogen bondings, Bitumen, Mechanical properties, Organogel

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Cavitation in mesoporous materials

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Abstract

Porous materials applications are wide and range from gas storage to chemical catalysis. Their characterization is essential and usually done through the analysis of the evaporation process in the imbibed material. Depending on temperature and the geometry of the pores, evaporation can occur *via* two mechanisms: meniscus recession or bubble nucleation, i.e. **cavitation**. The lattest is usually overlooked and can lead to incorrect characterizations for porous materials such as cage-like silicas.

Cavitation is supposed to occur in pores presenting an "ink-bottle" geometry, where cavities are connected through narrow enough aperture to the outer gas reservoir. When the cavities are wide ($>$ 10 nm), the cavitation threshold is expected to be consistent with the **classical nucleation theory** (CNT) [1]. We have recently found this to be true for hexane at room temperature in **porous alumina** (PoAl) [2]. However the threshold measured in **porous silicon** (PoSi) was much higher and dependent on the pore dimension and length . As a similar result was observed with nitrogen at 77 K [3], it motivated systematic studies in temperature on PoAl and PoSi with **nitrogen**. Overall, we find that the cavitation thresholds are in good agreement with the CNT predictions. However we observe a systematic deviation at low temperature probably due to the high curvature of the bubbles. Furthermore, the study of cavitation in narrow pores showed the first indication of confinement effects.

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Doebele, V.; *et al.* PRL **2020** *125*

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Keywords: cavitation, bubble, surface tension, nitrogen, porous material

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STRUCTURE/PROPERTY RELATIONSHIPS OF ALGINATE-BASED INJECTABLE HYDROGELS

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Abstract

Watersoluble thermoresponsive polymers have been the focus of intensive research in the last decades as they found applications in very different areas like oil recovery, food industry, cosmetics and a growing trend in medicine. Indeed, when such systems are able of generating a sol-gel transition under physiological condition, this opens the way to important developments in biomedical applications such as controlled drug release or tissue engineering by means of injectable matrices.

In this context, thermoresponsive copolymers designed with responsive macromolecular sequences, characterized by a Lower Critical Solution Temperature (LCST) close to physiological conditions, are promising candidates for injectable systems. In the case of such application, the important specifications are the injectability of the solution at room temperature and the behavior of the physical network formed at body temperature which is characterized by its viscoelastic and adhesive properties, as well as its ageing behavior in a wet environment.

Based on previous works, a series of graft copolymers based on an alginate backbone grafted with thermoresponsive side-chains has been designed. Different types of thermosensitive side-chains have been used, like poly(*N*-isopropylacrylamide) (PNIPAm), poly(oligo(ethylene glycol) methyl ether methacrylate), etc. With this versatile architecture, we can modify at will either the molar mass of the backbone, as well as the nature and/or the grafting density of the LCST side chains. In this presentation, we will emphasize the relationships between the copolymer structure and the thermoresponsive properties investigated by swelling, rheology, injectability and tack experiments.

Release studies of a model drug will also be presented.

Keywords: Hydrogel, LCST, PNIPAM

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*Speaker

Towards hybrid porous solids (MOFs) integration for cultural heritage preservation

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Abstract

Recent cultural heritage artefacts (visual and audio memories) have been found to be at risk of degradation on the accounts of the natural instability of their main component, cellulose acetate (CA). This phenomenon results mostly from the released acetic acid, that will have an autocatalytic effect increasing constantly the level of degradation. One low-energy method implemented to hinder this process consist on the use of adsorbents for selective acetic acid capture[1-4]. However, the relative humidity in archives can be above 40%, impairing the use of the commercially available hydrophilic sorbent options. This is the case for zeolites where water will compete with acetic acid for the available adsorption sites. Metal-Organic Frameworks (MOFs), a class of hybrid crystalline porous solid materials[1], [2] with unprecedented features (porosity, surface , flexibility, open metal sites...).[3], have shown promising interactions with acetic acid, decreasing the levels of this compound inside a closed chamber.[4] However, the selectivity was attributed to the use of functionalized expensive organic linker, hampering the potential use as a conservation strategy in collections. For this use, green and cheap-linker based MOF that shows high acetic acid adsorption performance is required. In addition the fulfillment of this requirements, can also lead to other high industrial interest applications. However, few studies have been conducted showing MOFs industrial potential. This can be achieved with a complete cost estimation, which has been already reported.[5] Following this method pilot scale evaluation of the synthesis is necessary. Furthermore, for the incorporation of this materials, macroscopic mechanically stable particles are needed, in order to avoid loss of material that can damage the artefacts. Therefore, the main objectives of this study is the synthesis of performant MOFs for cultural heritage preservation, optimization and scale-up, shaping, and evaluation of the economic potential by means of production cost estimation.

Keywords: Metal, Organic Frameworks, Films Preservation, Selectivity, Acetic acid

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*Speaker

MICROMECHANICS AND MOLECULAR INTERPRETATION OF CAVITATION IN SOFT POLYMER LAYERS

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Abstract

Every second, 29 Tb of data are produced on the internet, stocked and exchanged between continents. The vast majority of that data transits via optical fibres, consisting of thin glass fibres which carry light over hundreds of kilometres by total internal reflection. Being exposed to extreme conditions, these fibres are protected by several layers of polymers and metal. The first layer of protection consists of a soft elastomeric acrylate resin. This thin coating is under variable hydrostatic pressures created for example during manufacturing and during use. This may lead over time to the formation of cavities and ultimately to fibre blindness. The mechanisms ruling the nucleation and growth of cavities depend on various material parameters. Several models have been proposed, suggesting that the cavitation resistance is directly linked to the Young modulus(1) or that it depends on the initial defect size(2). Experimental studies(3) however suggest a more complex cavitation behaviour where the network's fracture toughness and the strain hardening both play a role.
By UV polymerizing thin films consisting of a mix of di-acrylate-functionalized PPG8000 and 2 acrylate monomers (2-ethylhexyl acrylate and 2-phenoxy ethyl acrylate), and testing their behaviour under hydrostatic stress, the link between mechanical properties and cavitation resistance can be investigated. Through changes of oligomer functionalization and monomer ratios, different network architectures and properties can be achieved. The cavitation process is observed in a sphere against flat confinement. The opening of cavities in the thin layer is recognized by sudden drops of the force during the loading, while the end of the curve shows the final fracture of the sample.

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Keywords: Cavitation, Hydrostatic pressure, Acrylate network, UV polymerization

In the Search for the Best Solid Electrolyte-Layered Oxide Pairing for Assembling Practical All-Solid-State Batteries

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Abstract

The global trend towards to boost energy density of today's Li-ion batteries is generating considerable attention on all-solid-state batteries (ASSBs) that could fulfill the demand taking advantage of lithium-metal anode.1 However, such potential benefits are mainly plagued by interfacial decomposition reactions at electrode materials hindering highly performing ASSBs.2 Focusing on the positive electrode, interfacial challenges essentially hinge on nature of solid electrolytes (SEs) stemming from chemical/electrochemical incompatibility toward cathode composite components, which need to be addressed in cross-comparison.
Herein, we have studied the chemical/electrochemical compatibility of three inorganic solid ion conductors (β-Li3PS4, Li6PS5Cl, and Li3InCl6) as part of cathode composite paired with layered oxide cathode active material (LiNi0.6Mn0.2Co0.2O2, NMC622) in cross-comparison for designing highly performing ASSBs. The solid ion conductors were firstly prepared by solvent-assisted and solvent-free routes and latter their structure, morphology and electronic-ionic conduction were characterized by XRD, SEM and EIS spectroscopy. Moreover, cathode composites made of NMC622 and the synthesized Li+ conductors were further tested to benchmark their electrochemical cycling performances in full-solid-state batteries. Furthermore, we unraveled the cell performance limitations of studied cathode composites via characterization techniques. Overall, we hope this work guide to understand chemical/electrochemical challenges for achieving practical ASSB cells.

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Keywords: Solid, state battery, solid electrolyte, solvent, based synthesis, solvent, free synthesis, cathode composite

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Development of predictive approaches for biomolecular association kinetics

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Abstract

Atomistic computer simulations of rare events have three paramount goals: predicting detailed mechanisms, free energy landscapes, and kinetic rates. All of these tasks are, in many cases, cumbersome and require intensive human and computer effort, being the calculation of rates the most difficult. With this Ph.D. thesis, we propose to develop efficient methodologies for the calculation of transition rates and to apply them to an important problem: the association and dissociation of biomolecular complexes. Transition path sampling trajectories are the golden standard to access mechanistic information: we demonstrate that they also encode accurate thermodynamic and kinetic information, that can be extracted by training a data-driven Langevin model of the dynamics projected on a collective variable, allowing to recover free energies, position-dependent diffusion coefficients, and rates. On the other hand, enhanced sampling methods, such as metadynamics, can accelerate the sampling of rare events but they distort the dynamics. To overcome this limitation, we developed a method based on Kramers' theory for calculating the barrier-crossing rate when a time-dependent bias is added to the system, measuring at the same time the quality of the collective variables. The newly developed theoretical and computational tools will find application far beyond the field of biomolecular association, from chemical reactions in solution to the nucleation of inorganic materials, thanks to the strong similarity among the corresponding activated processes from the point of view of the dynamics of complex systems and of statistical mechanics.

Keywords: kinetic models, computer simulations, Langevin models

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Determination and benchmarking of 27Al(d, α) and 27Al(d,p) reaction cross sections for energies and angles relevant to NRA

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Abstract

In the present thesis, differential cross-sections of Al(d,p&α) reactions were measured, and the cross-sections were benchmarked with thick target spectra obtained from pure Al for the first time in two independent laboratories. The Al(d,p&α) differential cross-sections were measured between 1.4 and 2 MeV at scattering angles of 165○, 150○, and 135○ in the VDGT laboratory in Tehran (Iran), and the same measurements for detector angle of 150○ were repeated from scratch, including target making, with independent equipment on the SAFIR platform at INSP in Paris (France). The results of these two measurements at 150○ are in good agreement, and for the first time, a fitted function is proposed to describe the Al-cross sections for which no suitable theoretical expression exists. The obtained differential cross-sections were validated through benchmarking, by fitting with SIMNRA deuteron-induced particle spectra obtained from a high purity bulk Al target at both labs for deuteron incident energies between 1.6 and 2 MeV. The thick target spectra are well-reproduced. The evaluated and benchmarked cross-sections have been uploaded to IBANDL.

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benchmarked with thick target

Keywords: differential cross, sections, Al(d, p&α) reactions, benchmarked with thick target

Toward new porous materials for the capture of interior odors

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Abstract

Volatile Organic Compounds (VOCs) are one of the main pollutants of car cockpit. Some of them, can be responsible for health issues such as irritation of the respiratory system, headache and other symptoms. All together, they are called "Sickening building syndrome. Some of them are odorant, which can provoke discomfort for the passengers. Hence, customers became more aware of the danger of these compounds especially in Asian countries (China and Korea). Indeed, they are, so far, the only countries where VOCs are regulated inside the car cabin. A car with no odor, has become for them synonymous of a safe car.
Thus, the new trend is to get rid of VOCs inside the cabin. Up to now, the solution used is a filter composed of activated carbon. Activated carbon are cheap materials, rather versatile, which show an overall good performance for the capture of apolar VOCs such as aromatics. However, they have proven to be limited due to a lack of selectivity and desorption when the temperature increases. The latter is one of the most problematic when it comes to car especially when it is parked during summer time. Indeed, all or a part of the VOCs captured by the filter could be released and deteriorate even more the air quality of the cabin especially when the users would enter the car.

In this regard, Metal-Organic Frameworks (MOFs) has aroused as potential candidates to replace activated carbon, Their high degree of modularity in terms of structural and physiochemical feature, can allow to find suitable candidates for many different applications, in particular for gas/vapor capture and/or separation.
The goal of my PhD financed by Stellantis is to understand the key parameters governing the adsorption between MOFs and VOCs and determine the best solution (single or mixed materials) to adsorb cocktail VOCs.

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Keywords: MOFs, VOCs, air quality, adsorption, automotive cockpit

Formulation of self-healing anode composites for lithium-ion battery. Study of potential polymer structures for electrode assembly

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Abstract

The increase in storage capacity and cycle life performance of Li-ion batteries are on demand for building enhanced electronic devices. In this regard, silicon stands amongst the most promising candidates for advanced anode materials in Li-ion batteries owing to its high theoretical storage capacity of c.a. 3600 mAh.g-1, which is almost ten times higher than the commercialized graphite anodes. Nonetheless, the envisioned higher storage capacity through the replacement of graphite by silicon as active matter comes with defeating poor cyclability and weak storage capacity retention. These drawbacks originate from the electrochemical lithiation of silicon, which experiences colossal volume variations (_˜300%) leading to the electrode structural collapse and thus poor cycling performances. In the midst of the strategies devoted to Si electrode cyclability we focus here on the design of Si anode binders that are responsible for maintaining the electrode structure and accommodating the mechanical stresses along with cycling. These binders are able to form reversible bonds with Si surface, allowing the healing of cracks that form in the electrode composite during charge and discharge cycles. Along with these lines, specific molecular design principles are implemented to obtain polymeric binders that show healing activity; high stiffness; elasticity; adhesion; ionic conductivity; electrochemical stability and electrolyte absorption. This work should therefore contribute to the current state-of-art of binders for negative silicon electrodes and allow the increase of the energy storage capacity in lithium-ion batteries.

Keywords: Si anodes, binders, copolymers, adhesion, healing

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Self-healing vitrimers for soft robotics

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Abstract

Soft robotics is an emergent branch of robotics, which involves incorporation of elastomeric elements. Addition of soft materials into robotic devices allows better flexibility and adaptability to the environment than when robots are made of hard and rigid components. However, the soft components are susceptible to damage, which can lead to the loss of the robot functionality. Therefore, it is advantageous to use self-healing (SH) elastomers to prolong the soft robot's lifetime. In all cases, a trade-off between self SH ability and mechanical properties is unavoidable. To overcome this dilemma, we combine physical hydrogen bonds and exchangeable ester bonds, which are responsible for good self-healing and mechanical properties, respectively. To detect a material damage (and possibly start a healing process), a soft robot must be equipped with a sensing system such as strain sensors. Therefore, we integrate piezo-resistive strain sensor fibers into the elastomeric materials by a so-called "sandwich-welding" technique. This work leads the way to a fully autonomous soft robot, which is able to detect and repair any damage of its soft components.

Keywords: self healing elastomer, soft robotics

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Action mechanisms of admixtures in mineral binders of low Portland cement content

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Abstract

With four billion tons produced each year, Portland cement is the most used manufactured material in the world. However, its production by calcination of limestone and clay leads to very high CO2 emissions [1]. One way to mitigate this effect is to use industrial wastes as primary materials. In particular, ground-granulated blast-furnace slag, a by-product of the steel industry, can be hydrated with alkali solutions to make a binder with similar properties as Portland cement. Still, one major hindrance remains to its use at a large scale. Indeed, to cast and pump properly cements, a high and time-controlled fluidity is needed.

Our objective is thus to first understand the hydration reactions taking place in alkali-activated slag cements depending on the chemistry of the activators. This is then correlated to the rheological behavior of the fresh pastes. This work thus relies on a vast range of analysis techniques such as Nuclear Magnetic Resonance spectroscopy, X-ray diffraction, thermal analysis, calorimetry, rheology and chemical analysis.

The first results show that the type of hydrates formed and the reaction kinetic depend on the activators used. Moreover, this affect the rheological behavior of the paste with a quick stiffening in some cases. Finally, this new information will help us find ways to control the fluidity of the cement over time with the use of chemical admixtures.

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Keywords: Cement, Environmental friendy, Rheological behaviour, MAS NMR, XRD

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Numerical modelling of cavitation and fibrillation in PSA

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Abstract

In a pressure-sensitive adhesive (PSA) tape, adhesion rupture is accompanied by fibrillation and cavitation of the adhesive layer. In this study, we propose a multiscale picture of adhesion rupture, involving a better understanding of fibrillation and cavitation. Numerically, a single fibril is modeled using the Finite element method using axis-symmetric boundary conditions. An Arruda Boyce, hyperelastic constitutive law is employed to tackle the large strains associated with the computer modeling of the layer of adhesive. Apart from Arruda Boyce, we are using other relevant constitutive relations like the Yeoh model, as well. We found that peeling a single fibril from a bulk of adhesive requires more energy than the uniaxial extension of the fibril for the same patch diameter in the numerical study, which is true for peeling experiments previously done at the SIMM lab. [1] In addition to that, we are also studying Cavity expansion along with the fibril extension and we want to connect these two phenomena happening in PSAs by numerical study. Our final aim is to connect the macroscopic work of fracture and the dissipative properties of the PSA material through a proper description of the large strain deformation of the interface.

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Chopin J.; Villey R.; Yarusso D.; Barthel E.; Creton C.; Ciccotti M., Macromolecules 2018, 51, 21, 8605–8610

Keywords: Cavitation, Fibrillation, PSA

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