JED 397: Les Journées de l'Ecole Doctorale 397

2-3 Nov 2023
Paris
France

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Tuning the Hydrophilicity of the Electrochemical Interface to Modulate the Oxygen-Atom Transfer in Electrocatalytic Epoxidation Reactions

Florian Dorchies * [1], Alexis Grimaud [1,2]

[1] Laboratoire Chimie du Solide et Energie (CSE) – CNRS : UMR8260 – 11 Place Marcelin Berthelot, 75005 Paris, France
[2] Grimaud Research Group – 2609 Beacon street 201 Merkert Chemistry Center Chemistry Department, Boston College 02467, Chestnut Hill, MA, United States

Electrosynthesis is foreseen as a viable synthetic route to replace energy intensive thermal synthesis owing to its innate sustainability and its ability to perform chemoselective functionalization of C-H and C=C bonds. Among the accessible chemical functions, the synthesis of epoxides is crucial as they serve as building blocks in organic chemistry and for industrial applications such as polymer synthesis. While heterogeneous electrochemical epoxidation methods currently rely on the *in-situ* generation of hazardous oxidizing agents such as Cl2, Br2 or H2O2, it was recently demonstrated that oxygen-atom transfer from water to C=C bonds to form epoxides could be achieved in hybrid acetonitrile (ACN)/aqueous electrolytes.1,2 Following this seminal demonstration, critical questions must be answered to improve the efficiency of the process. Among them, the role of the composition of the hybrid ACN/aqueous electrolyte on the selectivity and yield of the reaction must be unraveled. In this work, we studied the electrocatalytic epoxidation of cyclooctene at the surface of gold in ACN/aqueous mixtures.3 We show that the hydrophilicity of the electrode/electrolyte interface can be tuned by changing the nature of the supporting salt cation, hence affecting the reaction selectivity, while the bulk solvation structure of cyclooctene remains unaffected. At low overpotentials, hydrophilic interfaces formed by using strong Lewis acid cations (Li+ and Na+) are found to favor gold passivation. Instead, hydrophobic interfaces created by the use of large organic cations (tetrabutylammonium) favor the oxidation of cyclooctene and the epoxide formation. Our study directly demonstrates that tuning the hydrophilicity of electrochemical interfaces can improve both the yield and selectivity of anodic reactions at the surface of heterogeneous catalysts. More generally, we hypothesize that controlling the electrolyte structure in bulk and at the electrochemical interface could offer an additional degree of modulation in the design of new electrosynthetic methods.4

Keywords: Abstract

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[*] Speaker

Replacing polyurethane foam with reinforced agar gels

Perrine Pipart * [1], Guylaine Ducouret [1], Théo Merland [1], Yvette Tran [1], Dominique Hourdet [1]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) (SIMM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin 75231 PARIS CEDEX 05, France

Glycerol is widely used as a colligative cryoprotectant that raises the osmolality of body fluids and reduces the water available to form extracellular ice. It is also active in maintaining the structure of biological macromolecules and in promoting protein self-assembly through preferential hydration. Moreover, the Glycerol/Water (G/W) system is a mixture of choice if one wants to easily vary the viscosity of the fluid and the viscoelastic properties of polymer solutions and gels. In this work, we are interested in the mechanical & rheological properties of Agar gels in Glycerol/Water co-solvents. While agar is very well known for its gelling ability in water upon cooling, with the formation of double helices that self-assemble into fibrillar network, our goal is to understand the impact of the glycerol content on the sol-gel transition and ultimate material properties. For this purpose, we will report in this presentation the cold setting of agar networks in various G/W environments and describe their macroscopic properties, toughness, elongation at break, swelling at equilibrium and adhesiveness, in relation with the modification of the 3D structure.

Keywords: Mechanics, hydrogels, organogels, biopolymer

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*Speaker

Cationic Reversible Addition-Fragmentation chain Transfer - Ring Opening Polymerization (CRAFT-ROP) of 2-methyl-2-oxazoline

Solène Le Roux * [1], Véronique Bennevault [1,2], Philippe Guégan [1]

[1] Equipe Chimie des Polymères, Institut Parisien de Chimie Moléculaire (ECP, IPCM) – Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique – Sorbonne Université, 4 place Jussieu, 75252 Paris Cedex 05, France
[2] Université d'Evry-Val-d'Essonne (UEVE) – Université d'Evry-Val-d'Essonne – Rue du Père Jarlan 91025 Evry Cedex, France

Polyoxazolines are usually obtained through a cationic ring-opening polymerization (CROP) mechanism (1,2). It has been shown that a cationic reversible addition–fragmentation chain transfer (RAFT) polymerization mechanism can be considered to polymerize olefins such as vinyl ethers or styrene derivatives in the presence of transfer agent (3). RAFT polymerization is known to improve the control of polymerization and molar masses (3–5). While cationic RAFT polymerization of vinylic monomers is drawing large attention, no comparable investigation has been undertaken for heterocycles and in particular 2-alkyl-2-oxazolines.
Thus, several RAFT agents were investigated to synthesize poly(2-methyl-2-oxazoline)s but one CTA has been selected as it was able to react with the oxazolinium active centers. The amount of RAFT agent involved was studied to show its influence on the molar mass of the formed polymer and kinetic studies were performed. A CRAFT-ROP mechanism could therefore be established by analogy with the radical one (4). The polymers structures were characterized by 1H, 13C, COSY, HSQC and DOSY NMR and the chain ends assessments were achieved by MALDI-ToF. Finally, the molar masses were evaluated by SEC.

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[*] Speaker

Keywords: Cationic Reversible Addition Fragmentation chain Transfer, Cationic Ring Opening Polymerization, 2, oxazoline polymerization

Peptide-polymer bioconjugate synthesis: toward the modulation of the self-assembly properties of amyloid-β peptides

Emma Mongkhoun *† [1], Philippe Guégan [1], Nicolas Illy [1]

[1] Institut Parisien de Chimie Moléculaire (IPCM) – Chimie Moléculaire de Paris Centre, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR8232 – Sorbonne-Université, 4 place Jussieu 75252 Paris Cedex 05 Bâtiment F/74, France

Peptides are powerful macromolecules, highly bioactive, capable of biorecognition, stimuli responsive, biodegradable with a low immunogenicity (1). They have been investigated for therapeutic approaches, and hundreds of peptide-based drugs are available on the market or under clinical trials (1-2). However, native peptides also have weaknesses affecting their initial properties and pharmaceutical potential: chemical instability, rapid *in vivo* degradation and physical instability (e.g. fibrillation). Aggregation phenomena have significant health consequences and are implicated in neurological diseases, such as Alzheimer and Parkinson (3).
Polymer-peptide conjugates combine the functions and properties of biomolecules and synthetic polymers in a single hybrid material (4). Synthetic polymers are less complex but chemically more diverse and have complementary properties: e.g. solubility in aqueous or organic media, stability to T○ or pH, mechanical strength, elasticity or melt processability.

We propose to use the peptide bond as initiator for the synthesis of polymer-peptide conjugates. The amide bond is universal being the only chemical moiety on all peptide residues. Our group developed a one pot two-steps method to initiate the polymerization of episulfides using primary amine and N-acetyl homocysteine thiolactone (NHTL) as initiating system (5). In a first part of this work, the selectivity of the amino-acid thiolation with NHTL has been investigated. Then, the propylene sulfide AROP has been performed on amino-acid/NHTL systems. A library of amino-acids and short peptides have been successfully functionalized with poly(propylene sulfide) using NHTL as a co-initiator through a "grafting-from" strategy.

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[*] Speaker

[†] Corresponding author: emma.mongkhoun@sorbonne-universite.fr

Keywords: Bioconjugates, peptide, polymer, AROP, thiolactone, episulfide, poly(thioether), amyloid, aggregation

Rational selection of sodium layered oxides for high performance Na-ion batteries

Elisa Grepin * [1,2,3], Ivan A. Moiseev [4], Artem Abakumov [4], Jean-Marie Tarascon [1,2,3], Sathiya Mariyappan [1,3]

[1] Collège de France - Chaire Chimie du solide et énergie – Chimie du solide et de l'énergie – 11 Place Marcelin Berthelot, 75231 Paris, France
[2] Sorbonne Université – Sorbonne Université – 4 Place Jussieu, 75005, Paris, France
[3] Réseau sur le stockage électrochimique de l'énergie (RS2E) – Aix Marseille Université, Université Toulouse III - Paul Sabatier, Université de Haute-Alsace (UHA) Mulhouse - Colmar, Collège de France, Ecole Nationale Supérieure de Chimie de Paris - Chimie ParisTech-PSL, Université de Pau et des Pays de l'Adour, Institut de Chimie du CNRS, Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique, Institut National Polytechnique (Toulouse), Institut Polytechnique de Grenoble - Grenoble Institute of Technology, Nantes Université, Université de Montpellier, Ecole Nationale Supérieure de Chimie de Montpellier – 33 rue Saint-Leu - 80039 AMIENS CEDEX 1, France
[4] Skolkovo Institute of Science and Technology [Moscow] (Skoltech) – 3 Nobel Street, Moscow, 121205, Russia

Sodium ion batteries (NIBs) are gaining importance as an energy storage technology complementary to the Li-ion batteries. In this regard, sodium-based layered oxides are recognized as one of the most suitable positive electrode candidate for NIBs, but vast variety of their chemical compositions and crystal structures complicates the selection of the best material. Indeed, O3-type phases are known to exhibit higher capacity while P2 phases are sodium deficient and show better power rate capability. To shed light on different figures of merit that control the selection of layered oxide material for NIB applications, we compare here a P2, P2-O3 intergrowth and two O3 sodium layered oxides composed of the same transition metals (Ni, Mn, Ti and Zn) but in differing stoichiometries. The results show that the new P2-type Na0.67Ni0.3Zn0.03Mn0.52Ti0.15O2 phase reported here combines most of the advantages, such as stability towards moisture, reduced surface reactivity, better thermal stability and high rate capability, which are essential for commercialization, except for a limited capacity (_˜125 mAh/g) compared to the O3 NaNi0.45Zn0.05Mn0.4Ti0.1O2 phase (_˜180 mAh/g), reported by our group previously. Altogether, this work enlarges the family of attractive Na-based positive electrodes and teaches us that we should not solely be obsessed with the capacity of a material to decide of its applicability.

Keywords: Sodium ion batteries, sodium layered oxides, P type and O type structures, cycling stability, surface reactivity

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[*] Speaker

Colloidal Carbon Quantum Dots for More Stable Perovskite Solar Cells

Dongjiu Zhang * [1], Zhelu Hu [1], Chenghao Xin [1], Jiazhuo Nie [1], Lionel Aigouy [1], Laurent Billot [1], Zhuoying Chen† [1]

[1] LPEM – LPEM, ESPCI Paris, PSL Research University, Sorbonne Université, CNRS – France

Organic-inorganic hybrid perovskite solar cells (PSCs) have exhibited excellent photovoltaic performance comparable to conventional silicon solar cells, except for their non-negligible poor long-term stability induced by various environmental factors (e.g., moisture, oxygen, and ultraviolet (UV) light). In particular, the perovskite absorber layer has been found to undergo various degrees of degradation due to UV radiation. To address this issue, in this work, we investigate the possibility to harvest the unique optical property of colloidal carbon quantum dots (CQDs) on perovskite solar cells. To this aim, uniform UV absorbing and visible emitting CQDs were synthesized. Thorough structural and optical characterizations were performed on them. Finally, they were applied onto functional perovskite solar cells as a UV protection and down-shifting layer and we studied the effect of CQDs on the degradation behavior of the solar cells under UV illumination. Under an identical UV degradation condition, optimized CQD-protected perovskite solar cells exhibited only 5% of PCE drop after 100 hours of UV exposure (in air) in comparison to control devices (without CQDs) which exhibited $>$ 50% of PCE drop after 40 hours.

Keywords: CQDs, Perovskite Solar Cells, Stability

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[*] Speaker

[†] Corresponding author: zhuoying.chen@espci.fr

Chitosan grafted with fibronectin as a building unit for bioactive thermosensitive hydrogels

Pierre Marquaille * [1,2], Emmanuel Pauthe [2], Laurent Corte [1,3], Sophie Norvez [1]

[1] Chimie Moléculaire, Macromoléculaire et Matériaux (UMR7167) (C3M) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin 75005 Paris - Bat E 3ème étage, France
[2] Equipe de recherche sur les relations matrice extracellulaire-cellules (ERRMECe) – Fédération INSTITUT DES MATERIAUX DE CERGY-PONTOISE – Maison Internationale de la Recherche, Laboratoire ERRMECe, Rue Descartes 95000 NEUVILLE SUR OISE Cedex, France
[3] Centre des Matériaux (CDM) – Mines Paris - PSL (Ecole nationale supérieure des mines de Paris), Centre National de la Recherche Scientifique – Centre des matériaux - Pierre-Marie Fourt - 10 rue Henri Desbruères 91003 EVRY CEDEX, France

Chitosan (CS) solution buffered with sodium β-glycerophophate (βGP) is a thermosensitive solution having a gelation point above 37∘C, a property interesting for cell encapsulation and delivery using 3D scaffolds. Recently, a formulation platform using βGP and ammonium hydrogenophosphate (AHP) has been developed, providing cytocompatible macroporous hydrogels having both physiological pH and osmolarity. However, these hydrogels exhibit a poor bioactivity, which is attributed to the lack of interactions between the cells and the chitosan scaffold. This issue could be overcome by decorating the surface of the macropores with adhesion proteins, such as fibronectin (Fn). In this work, we propose to graft CS (Mw 250 kDa) onto Fn (Mw 550 kDa) using carbodiimide chemistry, leading to CS-*g*-Fn. Both the CS-*g*-Fn hydrogel and non-modified CS hydrogel exhibit similar gelation kinetics. Using fluorescently labelled species, CS* and Fn*, we compared the morphologies of CS hydrogels containing CS grafted onto Fn (CS*-*g*-Fn*), and CS hydrogels simply mixed with Fn (CS*+Fn*). Confocal microscopy observations show that both macromolecules are colocalized in the CS*-*g*-Fn* sample, whereas they are not in the CS*+Fn* one. Such a colocalization was confirmed quantitatively by comparing the Pearson's correlation coefficient for both samples. Image analysis using the morphological sieve technique also show that the CS-*g*-Fn hydrogel exhibits larger macroporosities than the non-modified CS hydrogel. Bioactivity was assessed by encapsulating Tomato(+)-MPNST cells in CS or CS-g-Fn hydrogels. After 96h culture, a significant number of cells presented more cytoplasmic extensions in the CS-g-Fn hydrogel than in the CS hydrogel, showing the efficiency of Fn grafting for biofunctionalization.

Keywords: Thermosensitivity, Hydrogel, Biofunctionalization, Cell encapsulation

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*Speaker

Efficient power density amelioration strategy for capacitive salinity-gradient and pH-gradient energy harvesting systems

Nan Wu * [1], Youcef Brahmi [1], Annie Colin† [1]

[1] Matériaux Innovants pour l'Energie (MIE) – Chimie-Biologie-Innovation (UMR 8231) – ESPCI, 10 rue Vauquelin,Paris F-75005, France

Osmotic energy released from the mixing of dilute and concentrated solutions is a new source of renewable energy. Our team developed previously an efficient capacitive concentration cell by using one single membrane and two inexpensive carbon-based capacitive electrodes. Such system converts efficiently the osmotic energy into electricity. It is safe, sustainable and environmental-friendly, but remains economically unviable today.

For power density amelioration, we developed a promising strategy by using an additional booster system in the circuit. The booster system generates an alternative electric voltage in phase with the period of flux reversal. The net power density output is calculated as the difference between gross power density dissipated and the power density generated by the booster system. We measured a maximal power density of 5.26 W.m-2 (salinity difference of 0.17 mol.L-1 and 5.13 mol.L-1), corresponding to a 59.8% increase compared with the value 3.29 W.m-2 without booster.

We extended this approach to processes involving solutions with pH gradients. These solutions are obtained by injecting CO2 from plant stacks into electrolytes such as Na2CO3 and NaHCO3. Under boosting strategy, we generated a higher net power density of 3.2 W.m-2 (pH gradient of 2.4) compared with the result of 1.7 W.m-2 reported in literature. A maximum net power density of 4 W.m-2 is obtained for a higher pH difference. In both situations, the process approaches economical viability.

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*Speaker

†Corresponding author: annie.colin@espci.fr

Redox coupling in glass: influence of antimony compounds on coloring and opacification

Léa Gardie *† [1], Laurent Cormier [2], Nadine Schibille [3]

[1] IMPMC (Institut de Minéralogie, Physique des Matériaux et Cosmochimie) – Sorbonne Université, CNRS, MNHN, IRD – France
[2] IMPMC (Institut de Minéralogie, Physique des Matériaux et Cosmochimie) – Sorbonne Université, CNRS, MNHN, IRD – France
[3] IRAMAT-CEB – Université d'Orléans, CNRS – France

Historically, multivalent elements have been used in the glass manufacturing in order to control its physicochemical properties. When several multivalent elements are introduced into the glass manufacturing process, they can interact with each other depending on the composition of the glass and the synthesis conditions. These differences in behavior between these multivalent elements are still poorly understood at the different stages of glass formation. Therefore, this work focuses more particularly on the role of antimony which can be used as an opacifier, decolorizer, or refiner in current industrial processes.

Glass opacification is a property sought since Antiquity for the manufacture of decoration or glass objects. This property can be brought by the presence of CaSb2O6 and Ca2Sb2O7 crystals dispersed in the glass matrix. Also, they can be added together with copper during the manufacturing process to bring turquoise coloring to the glass. The redox coupling between Sb and Cu can be a factor influencing the crystallization of calcium antimonates and therefore can be a determining factor in the choice of the crystallization process as well as the synthesis conditions. Understanding the interaction between antimony and copper is crucial to trace the manufacturing process of ancient glasses opacified and in the control of glass coloring.

The ancient glasses studied are white and turquoise mosaic tesserae dating from the 4th century AD (Villa Noheda, Spain). Glasses reproduced in the laboratory are synthesized from the composition of the Roman turquoise mosaic tesserae by varying the conditions of synthesis in order to compare the results with those of ancient tesserae. The analyses carried out by LA-ICP-MS, XRD, SEM-EDS and XANES spectroscopy will make it possible to determine the composition and the proportion of the crystalline phases, the microstructure, the rate of crystallization and to quantify the degree of redox of Sb.

Keywords: Glass, Redox, Opacification, Antimony, Roman tesserae

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[*] Speaker

[†] Corresponding author: lea.gardie@sorbonne-universite.fr

Micro-compartments of UCST hydrogels for microfluidic biotechnologies

Léa Milenkovic * [1], Thu Nguyen [2], Nadège Pantoustier [2], Yvette Tran [2]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France
[2] Sciences et Ingénierie de la Matière Molle (UMR7615), ESPCI Paris. – SIMM, ESPCI Paris, Université PSL, Sorbonne Université, CNRS – France

Thermo-sensitive polymers are of growing interest in many biomedical applications. The general idea of this project is to design hydrogel micro-compartments with UCST (Upper Critical Solution Temperature) polymers for microfluidic biotechnologies. Hydrogels can be actuated by temperature change to close/open micro-compartments or micro-cages to trap single cells for analysis (1). The thermo-actuable hydrogel is patterned and grafted on the bottom substrate of a microfluidic chip to form tens of thousands of micro-cages using photolithography. In the collapsed state, the micro-cages are opened, and in the swollen state, the hydrogel contacts the top substrate of the chip to close the micro-cages. Actuator technology based on UCST hydrogel micro-cages closed at 37○C, allows most of molecular biology operations under physiological conditions.
The challenge is thus to modify UCST polymers to form a hydrogel matrix based on thiol-ene click reaction, that can be micro-fabricated by Cross-Linking And Grafting (CLAG) (2), without leading sacrificing the thermo-sensitivity (Figure 1). As for the biological applications the polymers selected must not be very sensitive to saline solutions, the affinity of the polymer with water has to be governed by hydrogen bond interactions which can be finely tuned with temperature (T $<$ UCST: aggregation of polymers, T $>$ UCST: solubility of polymers).

We focus on acrylamide-based copolymers which can keep their UCST behavior in salt conditions. We synthesize the monomers and polymers that are used as elementary bricks for UCST hydrogels and study their thermo-responsive properties in aqueous and physiological solutions, such as poly(N-acryloylglycinamide)- or poly(N-methacryloylglycinamide)-based copolymers (3).

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[*] Speaker

Keywords: Thermostimulable, hydrogels, UCST polymers, microfluidic

Ecoresponsible Functional Antimicrobial Surfaces - SAFE

Laurence Gbaguidi * [1]

[1] Laurence GBAGUIDI (Doctorant 3e année) – Université Paris-Sorbonne - Paris IV – 11 Rue Alain Colas, France

SAFE aims to develop new robust, durable, industrializable and REACH compliant coatings with passive and/or active antimicrobial activity in order to fight against the formation and development of biofilms in air, water or confined environments. Indeed, the problems caused by the existence of biofilms impact many industrial sectors, resulting in a degradation of installations and their performance.In the literature, it has been established that a coating must have a low surface energy (between 15 and 25 mN/m), a low modulus of elasticity (0.002 - 0.5 GPa) as well as a molecular mobility on the surface (SAM and/or slippery surface) in order to obtain an antibiofilm effect. However, such prerequisites can pose problems in terms of durability (abrasion resistance - scratching). Our project aims at finding a compromise between low adhesion of microorganisms and durability. To do so, our strategy is based on the design of interpenetrated polymer-silicon derivative networks, the two components being linked at the nanometric scale. It is indeed possible to modulate some properties of these materials such as surface energy, elasticity modulus, abrasion resistance, adhesion properties by playing on the chemical compounds used, their relative proportion and the synthesis routes. In this study, we have realized coatings with variable surface energies and reduced modulus of elasticity (16 - 42 mN.m-1 and 2.8 - 8 GPa) . Regarding adhesion, we have performed compression shear tests according to ASTMD 5618 and biofilm growth experiments are under study with the LBBM. In parallel, more detailed analyses involving the measurement of the 1H spin-lattice relaxation time and 13C CP MAS NMR will allow us to access the dimension of phase nanosegregation in this type of material and the relative mobility of the species within the material, these two characteristics being important on the durability of the coatings and their antibiofilm action.

Keywords: coating, sol, gel, antimicrobial, eco, responsible

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*Speaker

Curie Composites NPs for failsafe Magnetocuring of resins

Naoures Hmili * [1], Ferdaous Ben Romdhane [2], Raju. V. Ramanujan [3],
Terry Steele [3], Souhir Boujday† [1], Juliette Blanchard‡ [1]

[1] Laboratoire de Réactivité de Surface (LRS) – Institut de Chimie du CNRS, Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique – Tour 54- 2ème etg 4 Place Jussieu - Case 178 75252 PARIS CEDEX 05, France
[2] Fédération de Chimie et Matériaux de Paris-Centre (FCMat) – Ecole Nationale Supérieure de Chimie de Paris - Chimie ParisTech-PSL, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique – 4, place Jussieu - Tour 54 75252 PARIS CEDEX 05, France
[3] Nanyang Technological University [Singapour] – 50 Nanyang Ave, Singapour 639798, Singapore

Adhesive Technology is attracting increasing interest from researchers for a range of emerging applications in sports, medicine, and industry. Traditionally, one-component adhesives are designed to cure using moisture, heat, or light. However, these methods are challenging to control and implement industrially. Herein, an approach to cure adhesives remotely is of high relevance. Our approach is based on Magnetocuring, where Magnetic Nanoparticles (MNPs) are introduced into adhesives and exposed to an Alternating Magnetic Field (AMF). Under AMF, the heat generated by MNP triggers the polymerization and curing of the adhesives (ex. Epoxy resin) (fig.1) Also, self-regulating heating can be achieved by adjusting the Curie temperature (Tc), i.e. Temperature above which the material loses its permanent magnetization, of the MNPs.

In this project, we synthesized a library of ferrite NPs (MnxZn1-xFe2O4) of various sizes (10 nm – 22 nm) and compositions (x = 0.5 – 0.9)(1), (2) which were characterized by TEM, XRD and EDX. Some of us have established that this library of MNPs offers a range of Tc and Specific Absorption Rate (SAR, i.e., their heating ability) suitable for magnetocuring of adhesive without overheating (2).

For magnetocuring, MNPs must be homogeneously dispersed in the resin at low concentration to preserve its mechanical properties. Therefore, we have worked on obtaining a colloidal MNPs suspensions by optimizing their stabilization with citrates. We have also worked on their coating with a silica shell of different thicknesses, which will serve as primer for further functionalization with silanes bearing different (R) groups to allow dispersion in water and/or organic liquids.

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*Speaker

†Corresponding author: souhir.boujday@sorbonne-universite.fr

‡Corresponding author: juliette.blanchard@sorbonne-universite.fr

Keywords: Magnetic Nanoparticles, synthesis, functionalization, coating, magnetocuring

Study of the yellow coloration of stained glass - focus on the amber chromophore

Déa Jais * [1], Laurence Galoisy [1], Georges Calas [1], Claudine Loisel [2]

[1] Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC) – Sorbonne Université, CNRS, Museum National d'Histoire Naturelle, IRD – 4 place Jussieu, 75005 Paris, France
[2] Laboratoire de recherche des monuments historiques (LRMH) – Centre de Recherche sur la Conservation – 29 Rue de Paris, 77420 Champs-sur-Marne, France

Yellow hues can be obtained in glass using various chromophores. From Roman times to the present day, glass colorants have evolved, from amber color due to a sulfur-iron complex to the bright yellow of CdSSe quantum dots through silver yellow given by surface plasmon resonance of metallic silver nanoparticles. The evolution of coloring has been made possible by the discovery of new raw materials and new processes, but some very old techniques have survived and are still used today.

The amber chromophore is one such method that appeared in antiquity and is still widely used today for stained glasses but also for UV-protective bottles and flasks. Studying this chromophore allows a better understanding of the color of stained glass and a better knowledge and control of the production of the industrial production. However, studying this chromophore in stained glass has long been complicated. Indeed, iron and sulfur are often present in these glasses as impurities, whatever the color of the glass. Only very precise redox conditions make it possible to obtain the yellow-amber coloration. In addition, a very low concentration of iron and sulfur is necessary to give the yellow color. Thus, chemical analysis is not sufficient to determine the coloring.

The spectroscopic methods and in particular the optical absorption spectroscopy take then all their sense for this study: it is very efficient even for very low concentrations and allows to study the charge transfer responsible for the color. For the stained glasses, the use of portable optical spectroscopy allows to quickly identify the yellow chromophore without damaging the stained glass. Raman and EPR spectroscopy were also used to better understand the structure and the very specific oxidation state of the amber chromophore.

Keywords: silicate glasses, color, spectroscopy, cultural heritage, redox

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[*] Speaker

Towards a Topological Insulator in 2D Lead Layers on Silicon Carbide

Axel Malécot * [1], Geoffroy Prévot† [1], Marie D'angelo‡ [1]

[1] Institut des Nanosciences de Paris (INSP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne-Université, Case 840 4 place Jussieu 75252 Paris Cedex 05, France

Graphene has been widely studied over the past 20 years for its electronic properties, but its technological applications are limited by the absence of gap at room temperature. That's why heavier elements from Group IV have been used to form a honeycomb-like structure similar to graphene to induce a gap opening through spin-orbit coupling. This has led to the synthesis of Silicene and Germanene, which have larger gaps of 2 and 24 meV, but still not sufficient to neglect kT at room temperature. In this regard, lead is a promising candidate for opening a larger gap. One team has achieved such structure on Pd(111), but the metallic properties of the substrate limit characterization and applications. On the other hand, Silicon Carbide (SiC), a wide-bandgap semiconductor, is predicted to be a suitable substrate for depositing lead to form a honeycomb structure with a topological gap, known as plumbene. According to calculations, this substrate would stabilize the topological phase, enabling the formation of a 2D topological insulator. In this context, we have studied the deposition of lead on different surface reconstructions of hexagonal Silicon Carbide (6H-SiC) in ultra-high vacuum. We have identified three new lead atomic structures on various surface reconstructions of the substrate, characterized by Low-Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and Scanning Tunneling Spectroscopy (STS). One of these lead phases exhibits a honeycomb-like appearance in STM and is the focus of our study. We propose an atomic model for these phases that is consistent with our experimental observations. These results open up prospects for the study of these topological states and their potential application in electronic devices, such as spintronics. However, challenges persist in the characterization and control of these new materials.

Keywords: 2D materials, Honeycomb structure, Scanning Tunneling Microscopy, Quantum Spin Hall effect

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*Speaker

†Corresponding author: geoffroy.prevot@sorbonne-universite.fr

‡Corresponding author: dangelo@insp.jussieu.fr

Bridging Chemistry, Physics, and Mechanics: Understanding How Blades Damage Chemical Bonds in Soft Materials

Donghao Zhao * [1], Alex Cartier [1], Matteo Ciccotti [1], Tetsuharu Narita [1], Constantino Creton [1]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) (SIMM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversiteéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin 75231 PARIS CEDEX 05, France

Soft materials have emerged as a novel class of materials with unique solid-like mechanical properties, making them promising candidates for a broad range of applications. Nonetheless, controlled damage, such as cutting, remains a critical requirement for soft materials. A lack of knowledge of the physical processes occurring during cutting poses a significant challenge for researchers, who must develop new methods to investigate the nonlinear geometry and deformation behavior of soft materials during cutting, to provide better solutions for controlled damage. Addressing these challenges requires a thorough understanding of the underlying physical mechanisms, necessitating interdisciplinary collaborations between materials science, mechanics, and physics. To describe the pure-shear cutting process of soft material, we employ a combination of chemical and mechanical methods to validate the assumption of the cutting damage zone. Furthermore, we study the nonlinear elastic zone surrounding the crack tip utilizing Digital Image Correlation. By analyzing the strain maps obtained from the DIC and damage map developed by mechanochemical tools and fitting them with theory, we were able to obtain a better understanding of the physical mechanisms involved in cutting soft materials. The damage zone at the crack tip can be detected by the fluorescent moiety caused by the scission-induced activation of the mechanophore. Compared with relatively broad and random damage areas damage zone (400 um) of the crack-propagation experiment, damage generated by a cutting tool exhibits a more concentrated and homogeneous nature. As the stretch ratio of cutting samples increases, these damage areas expand and evolve. These novel techniques present an exciting opportunity for us to develop a more comprehensive understanding of the mechanical behavior of soft materials during cutting. Ultimately, this research could lead to the development of more efficient and effective cutting methods for soft materials, with implications for a broad range of applications.

Keywords: Fracture mechanics, Soft materials, Cutting

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*Speaker

Cellulose-Alginate Hydrogels for Water Desalination Inspired by the Structure and Function of Plants

Katsuya Komiyama *† [1], Clémence Sicard [2], Francisco Fernandes‡ [3]

[1] Matériaux et Biologie (LCMCP-MATBIO) – Laboratoire de Chimie de la Matière Condensée de Paris – Sorbonne Université âĂŞ Tour 44-43 / Et.4 4, Place Jussieu 75005 PARIS, France
[2] Université de Versailles Saint-Quentin-en Yvelines, UMR 8180 – Université de Versailles Saint-Quentin-en-Yvelines – L'Institut Lavoisier de Versailles, 78035, Versailles, France, France
[3] Matériaux et Biologie (LCMCP-MATBIO) – Laboratoire de Chimie de la Matière Condensée de Paris – Sorbonne Université âĂŞ Tour 44-43 / Et.4 4, Place Jussieu 75005 PARIS, France

Plants have attracted enormous attention as biomimetic models because of their remarkable combination of mechanical strength and lightweight. The hierarchical cellular structure of highly-oriented cellulose fibrils in the matrix (hemicellulose and lignin) is largely responsible for such properties in plant tissues. Beyond the structural aspects, plants perform a myriad of functions. In particular, liquid transport between the roots and the leaves is inspiring to design new desalination devices. The driving force behind this function is transpiration, which determines water transport from the roots through the stems' macropores (xylem) up to the surface of its leaves, driven by sunlight. One of the consequences of transpiration is the separation of the water from its solutes. Especially, plants like mangroves, willows and reeds are able to generate clean water from seawater and wastewater through the solar power as a sole inexhaustible energy source. Here we propose an analogous system able to reproduce the functions and structure of the plant stem and leaves, ultimately capable of water desalination via sun-powered evaporation. The isotropic hydrogels corresponding to the "stem" were obtained by ice templating, a materials processing technique that enables the formation of aligned macropores by precisely controlling ice growth in solutions and/or suspensions. By freezing oxidized cellulose dispersion in alginate matrix and stabilizing them through ion-crosslinking, we aim at reproducing the vascular structure and function of the plant stem. Furthermore, buckypapers (carbon-clay black paper-like material) were prepared to act as artificial "leaves" by vacuum filtration (3), and placed on top of the anisotropic hyrogels. Because buckypapers have excellent photo-thermal properties, they accelerate the capillary liquid transport behavior of the hydrogels in the presence of the artificial solar light.

Keywords: cellulose, alginate, ice, templating, hydrogel, capillary action, desalination

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*Speaker

†Corresponding author: katsuya.komiyama@sorbonne-universite.fr

‡Corresponding author: francisco.fernandes@upmc.fr

Egg-tempera paint: formulation, drying and ageing

Floriane Gerony [*] [1,2]

[1] Laboratoire d'Archéologie Moléculaire et Structurale – Université Pierre et Marie Curie - Paris 6, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – France
[2] PHysicochimie des Electrolytes et Nanosystèmes InterfaciauX – Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – France

F. Gerony, L. de Viguerie, A.-L. Rollet, L. Michot, G. Mériguet & M. Jaber

Between the 13th and 15th centuries, in Italy, egg-*tempera* painting was the predominant technique before being superseded by oil paint. This practice consists in mixing pigments with an aqueous binder, in this particular case, egg yolk. Egg yolk is mainly composed of about 50% water, 30% lipids and 15% proteins (1). The paint's fate can be broken down into 3 main stages: formulation, drying and ageing, during which pigment-binder interactions play a major role (2).

Ancient recipes have been collected in order to reconstitute paints in the laboratory according to medieval processes. Their properties (texture, stability, preservation) differ according to the ingredients and their proportions. Rheological characterization shows that our reconstructions have a shear thinning behavior. During the first few hours after application on a support, water evaporates. NMR relaxometry enables to follow transversal relaxation of 1H protons (corresponding to lipoproteins and water protons) during drying (3). In the days and years that follow, up to hundreds of years, the paints continue to undergo several molecular changes. The ageing process is simulated by photodegradation under visible and UV light. Oxidation of lipids has been detected, strikingly reminiscent of the ageing mechanisms of oil paints (4).

Acknowledgements: This study was funded by the Observatoire des Patrimoines de Sorbonne Université (OPUS).

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[*] Speaker

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Molecular adsorption on Dumbbell Silicene

Laurita Florean * [1,2], Yves Borensztein [1], Hervé Cruguel [1], Romain Bernard [1], Fabrice Bournel [2], Geoffroy Prévot [1]

[1] Institut des Nanosciences de Paris (INSP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne-Université, Case 840 4 place Jussieu 75252 Paris Cedex 05, France
[2] Laboratoire de Chimie Physique - Matière et Rayonnement (LCPMR) – Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – 11 Rue Pierre et Marie Curie 75231 Paris Cedex 05, France

Following graphene discovery, 2D materials attracted rising attention due to their remarkable properties. Among them, silicene has been particularly studied as Si is essential in semi-conductor industry. Silicene presents an electronic structure very similar to the one of graphene, but is more sensitive to chemical environment. The possibility of tuning the electronic properties of silicene by molecular adsorption associated with the 2D geometry makes it a promising candidate for highly sensitive molecular sensors.

We have recently proven the existence of Dumbbell Silicene (DBSi) which shows a low density of adatoms, on top of Si atoms of the silicene layer, forming DB units. Adsorption of molecules onto these sites is expected to open a small gap in the electronic structure, while preserving the overall silicene band structure.

Using STM, we have followed the evolution of DBSi upon exposure to ammonia (NH3) and have noticed that depending on the temperature at which the experiment was carried out, the system behaved differently. At room temperature, if some molecules adsorb on top of DBs, other molecules are found to adsorb on the DB free regions silicene or on defects of the surface. On the other hand, at low temperature, we can spot a clear preference of adsorption of ammonia on top of DB sites as sought for the goal exposed above. Moreover, as expected by cooling down the sample, the physisorption is favored which lead to an increase of chemisorbed molecules too, that will stay fixed on top of the DBs once the sample is back to room temperature. The chemisorption is here in a competition with the desorption and happens only if the energy barrier is overcome. Therefore, at low temperature, for ammonia the DB sites are by far more reactive than the rest of the silicene layer.

Keywords: silicene, 2D, STM, XPS, vacuum, dumbbell silicene

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[*] Speaker

Oil removal by flowing of surfactant solution : a two scale approach

Marion Le Guevel * [1], Michael Levant [2], Valérie Molinier [3], Nicolas Passade-Boupat [2], Laurence Talini [4], FranÃğois Lequeux [5], Emilie Verneuil [5]

[1] Laboratoire Physico-Chimie des Interfaces Complexes – Sciences et Ingénierie de la Matière Molle (UMR 7615) – France
[2] Laboratoire Physico-Chimie des Interfaces Complexes (PIC) – Sciences et Ingénierie de la Matière Molle (UMR 7615) – ESPCI, 10 rue Vauquelin, 75005 Paris et Bâtiment CHEMSTARTUP, Route Départementale 817, 64170 Lacq., France
[3] Pôle d'Etude et de Recherche de Lacq [Total] (PERL) – TotalEnergies SE, Pôle d'Etudes et de Recherches de Lacq – Lacq, France
[4] Surface du Verre et Interfaces (SVI) – SAINT-GOBAIN, Centre National de la Recherche Scientifique – SVI UMR 125 CNRS/Saint-Gobain Recherche 39 quai Lucien Lefranc - BP 135 F 93303 Aubervilliers Cedex, France
[5] Laboratoire Physico-Chimie des Interfaces Complexes (PIC) – Sciences et Ingénierie de la Matière Molle (UMR 7615) – ESPCI, 10 rue Vauquelin, 75005 Paris et Bâtiment CHEMSTARTUP, Route Départementale 817, 64170 Lacq., France

During various industrial processes, porous media may be clogged by oil droplets. As a remedy, aqueous solutions of surfactants are generally injected in the media. The mechanism of the detachment of the oil droplets from the porous solid are not known and are the object of the present study.
We use a model system to mimic the phenomena that occurs in the porous media at one pore scale. We have selected a simple chemical system, which forms microemulsions at room temperature. The nature of the phase formed by a mixture of oil, water and the chosen surfactant depends on the water salinity. Addition of salt therefore result in very large variations of interfacial tension, from 10-2 to 20 mN/m.

In a previous study (1), it has been showed that the optimal detergency does not correspond to the salt concentration at which the minimum of interfacial tension is reached, but to a smaller concentration. We reproduced this phenomenon at the pore scale to understand the mechanisms that occur. We designed a microfluidic setup, monodisperse oil droplets are formed and further stuck on a borosilicate wall. A flow of aqueous surfactant solution is then imposed. The droplets detach above a critical shear rate. The contact line of the oil, salt water and borosilicate wall impact the detachment of the droplet. Thanks to the experimental observation, we understood that we needed to find a compromise between a low interfacial tension and a geometry of the drop which allow a good impact of the shear stress on the drop to have a maximum of detergency.

We also perform experiment above the critical micellar concentration to investigate the mechanism of dissolution of oil under flow.

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[*] Speaker

The systematic experiments performed in the microfluidic set-up shed new light on the mechanisms of detergency under flow.

Keywords: detergency, microfluidics, microemulsion

Understanding Clogging Mechanisms in Porous Media

Nathalie Santos De Pera * [1,2,3]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France
[2] Laboratoire de Physico-chimie des Interfaces Complexes (PIC) – ESPCI Paris, PSL Research University, TotalEnergies SE, Pôle d'Etudes et de Recherches de Lacq – France
[3] Pôle d'Etude et de Recherche de Lacq [Total] – Pôle dÉtude et de Recherche de Lacq [Total], Pôle dÉtude et de Recherche de Lacq [Total], Pôle d'Etude et de Recherche de Lacq [Total] – France

Produced Water Re-injection (PWRI) is a crucial process within the oil and gas industry that involves the reinjection of water extracted during oil and gas production back into reservoirs. This practice helps maintain reservoir pressure and reduce the water requirements. However, this water contains oil and residual particles that can aggregate and induce porous media clogging, causing a loss of injectivity. Water treatment can be technically challenging and expensive in order to meet injection standards. Thus, the objective is to better understand the underlying clogging phenomena to lead to a development of more efficient and cost-effective treatment. In the literature, clogging mechanisms are not fully understood, especially in the simultaneous presence of oil and particles. In this research, I present an experimental approach that mimics the PWRI process at microscopic scale with several pores and multiple oil and particles aggregates. Capillaries suspensions (i.e., solid particles aggregated by capillary oil bridges) are formulated to be injected into a 2D model porous media fabricated in a microfluidic chip. Pressure measurements and direct observations result in the determination of the kinetics of damage propagation inside the porous medium thanks to its transparency. Moreover, this setup has two principal advantages: first, it allows control of the physico-chemical parameters of the model produced water, such as oil and particles concentration, flowrates... Secondly, developing our own porous medium enables the variation of its geometric parameters (size, number, and geometry of pores, etc.). This parameters control is essential for studying factors influencing clogging phenomena and finally, for establishing a phase diagram to identify capillary suspensions passage regimes depending on experimental conditions.

Keywords: capillary suspension, porous media, clogging

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*Speaker

A novel millifluidics technique to generate monodisperse emulsions and study their separation dynamics

Andrei Zlobin * [1]

[1] Laboratoire Physico-Chimie des Interfaces Complexes (PIC) – Sciences et Ingénierie de la Matière Molle (UMR 7615) – ESPCI, 10 rue Vauquelin, 75005 Paris et Bâtiment CHEMSTARTUP, Route Départementale 817, 64170 Lacq., France

In crude oil, the presence of some components with a stabilizing effect generates inverse W/O emulsions. Their high stability leads to the appearance of a *dense-packed layer* (with a high volume fraction of water). Chemical additives accelerate the macroscopic separation of these emulsions. Performing the surfactant screening by bottle-test method, Dinh et.al. (1) have described a meta-stable state for such an emulsion along with developing a model of the emulsion separation dynamics with the droplet size distribution from 5 to 50 μm. But larger droplet sizes, higher viscosities and actual industrial systems conditions are yet to be verified within this theory.

In this research, a proposed millifluidics setup allows the creation of monodisperse emulsions with easily adjustable droplet sizes from 200 μm to 2 mm. One experiment includes two stages:

- The continuous dynamic stage is when the droplets arrive one by one and accumulate at the water-oil interface.
- The closed gravity separation stage is when only the coalescence of accumulated emulsion occurs.

A spatial-temporal distribution method (see *Figure*) is applied for experimental data analysis to describe the evolution of the interfaces and evaluate the coalescence rate.

The installation allows the control of the surfactant adsorption kinetics and, thus, to experiment in the non-saturated (by surfactant) concentration domain. Dodecane/water emulsions with varying quantities of Span 80 and Tween 20 were studied, and different separation regimes exist. The setup also simulates a sedimentation stage and emulsion droplet ageing (because of oil drainage) as in an existing separator unit.

Though the overall results exhibit a significative difference from Dinh's data (constant linear separation rate and no metastability observed), we provide an explanation of total droplet deformation proven by the droplet contact surface model.

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*Speaker

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Keywords: water, in, oil emulsions, millifluidics, coalescence, spatial, temporal distribution

Photoluminescence modulation of CdSe 2D nanoplatelets with CMOS-compatible bias operation

Huichen Zhang * [1], Victor Guilloux [1], Erwan Bossavit [1], Ningyuan Fu [2], Corentin Dabard [2], Sandrine Ithurria [2], Juan I Climente [3], Thierry Barisien [1], Emmanuel Lhuillier† [1]

[1] Institut des NanoSciences de Paris (INSP) – Sorbonne Université, UPMC, CNRS – France
[2] Laboratoire de Physique et d'Etude des Matériaux (UMR 8213) (LPEM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin, 75231 Paris cedex 05, France
[3] Universitat Jaume I – Spain

Nanocrystals, thanks to their broad spectral tunability and solution processability, appear as an appealing platform for the design of optoelectronic devices, such as light-emitting diodes, solar cells, and cameras. However, the light modulator is among the devices that remain unexplored, despite its wide applications in telecommunication, backlight in display, and biomedicine. Traditionally, achieving light modulation in confined heterostructures necessitates the application of a large electric field, which is incompatible with conventional CMOS electronics.

Here, we demonstrate efficient photoluminescence (PL) modulation in CdSe/ZnS 2D nanoplatelets in a photodiode stack, which is a new functionality of the device, and investigate the origin of the PL modulation. In a diode stack, the PL intensity of 2D nanoplatelets of CdSe/ZnS can be modulated reversibly over two orders of magnitude by applying reverse bias as low as 3 V. Such low driving bias ensures compatibility with CMOS operation.

To understand the origin of the efficient modulation of PL quantum yield (PLQY) in nanoplatelets under reverse bias, we combine the modeling of the electronic structure with time-resolved spectroscopy. While k.p. modeling shows that the radiative decay rate is reduced by 15% due to the spatial separation of wavefunction under bias, the overall PL decay rate increases by a factor of 4, suggesting the PL drop is dominated by a strong fastening of non-radiative decay. To further disentangle the effect of the electric field from charge injection, a capacitor model that excludes the charge injection is fabricated demonstrating no PL modulation, proving the efficient PL modulation is driven by charge injection.

Keywords: CdSe nanoplatelets, photodiode, photoluminescence, quantum, confinement Stark effect.

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[*] Speaker

[†] Corresponding author: el@insp.jussieu.fr

Coupling Ferroelectric to Colloidal Nanocrystals as a Generic Strategy to Engineer the Carrier Density Landscape

Mariarosa Cavallo * [1], Sylvia Matzen [2], Thomas Maroutian [2], Emmanuel Lhuillier† [1], Debora Pierucci [1]

[1] Institut des Nanosciences de Paris (INSP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne-Université, Case 840 4 place Jussieu 75252 Paris Cedex 05, France
[2] Centre de Nanosciences et de Nanotechnologies (C2N) – Université Paris-Saclay, Centre National de la Recherche Scientifique – 10 Boulevard Thomas Gobert, 91120, Palaiseau, France

In the context of nanocrystal-based optoelectronic devices for the infrared, the design of photodiodes faces a major challenge related to the identification of transport layers in vertical diode stacks, where a well-suited band alignment is required, as well as strategies for the control of the carrier density.(1) Alternatives to vertical diode stacks have already been proposed, for example multi-gated field effect transistors or coupling of NCs to bulk III-V semiconductors. Their main limitations are related to the continuous application of DC bias, which is required for gating: this consumes energy and introduces additional noise in the device.
The goal of my thesis is to explore a complementary alternative approach where the carrier density control can be achieved by coupling the nanocrystal layer to a ferroelectric material, by utilizing the remnant polarization of the latter and thus avoiding the need for gate bias application.
The idea is to use the up and down change in the ferroelectric polarization to directly form a lateral *p*-*n* junction in the nanocrystal film, as has already been achieved in the field of 2D materials.(2)

A first result has been obtained by designing a ferroelectric-NC heterostructure made of Lead Zirconium Titanate (PZT) and HgTe NCs. The effect of the ferroelectric polarization on the HgTe band offsets is revealed using nano-beam X-ray photoemission spectroscopy. A photodiode is then built and enhanced photoresponse and reduced noise are obtained thanks to the built-in potential of the diode.

However, while having the benefit of being a gateless/consumption-less strategy, production of such devices is limited by the fabrication process of the PZT (PLD, PFM writing...). Further efforts will be focused on finding methods compatible with larger substrate format.
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*Speaker
†Corresponding author: lhuillier@insp.upmc.fr

Keywords: optoelectronics, nanocrystals, infrared, pn junction, ferroelectric

Understanding the reactivity between Li1+xAlxTi2-x(PO4)3 and sintering aids to minimize densification temperatures in all-solid-state batteries.

Morgan Guilleux * [1], Arnaud Perez [1], Christel Laberty-Robert [1]

[1] Reactive Materials for Electrochemical Systems (LCMCP-RMES) – Sorbonne Universités, UPMC,
CNRS – Sorbonne Université âĂŞ Tour 44-43 / Et.4 4, Place Jussieu 75005 PARIS, France

All-solid-state batteries are considered as a promising candidate technology in the transportation field. By substituting the liquid electrolyte of standard Li-ion batteries with a solid electrolyte that conducts lithium ions, this new technology makes it possible to obtain higher energy densities (400 Wh/kg) and improve user safety. This system is composed of a negative electrode (metallic lithium), a solid electrolyte and a composite positive electrode. A critical point concerns the oxide solid electrolyte in the composite positive electrode. Indeed, the solid electrolyte must be densified by heat treatment ($> 900\circ$C) to approach its maximum ionic conductivity and form intimate contact with the active material. However, chemical reactivity of the solid electrolyte with the active material in the composite cathode has been observed as low as 700◦C for some systems. To prevent this reactivity, one strategy is to lower the densification temperature of the solid electrolyte by using lithium salts as sintering aids. However, these temperatures remain too high and close observation of powder X-ray diffraction data reported in the literature, confirmed by our own experimental results, show that resistive impurity phases such as LiTiOPO4 and Li4P2O7 already form at these temperatures. This work aims to explore chemical reactivity mechanism of specific lithium salts when interacting with the solid electrolyte Li1+xAlxTi2-x(PO4)3 (LATP) during densification and sintering process. Our work shows that the chemical reactivity between lithium salts and LATP is a limiting factor in decreasing the sintering temperature of the material below 700◦C. This new knowledge enables us to reexamine sintering of oxide ceramics and explore new paradigms to address this challenge.

Keywords: All solid state batteries, Oxide solid electrolyte, Densification and Sintering process, Chemical reactivity

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[*] Speaker

Ammonia removal using metal oxide nanoparticles deposited on activated carbon (AC/MO-NPs)

Ali Djellali * [1], Juliette Blanchard [2]

[1] LRS – Laboratoire de Réactivité de Surface (LRS-UMR 7197, UPMC-CNRS), Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, France – France
[2] LRS – Laboratoire de Réactivité de Surface (LRS-UMR 7197, UPMC-CNRS), Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, France – France

One of the main industrial air pollutants is ammonia (NH3), which damages ecosystems by eutrophication, acidification, and contamination of groundwater and soil. It can potentially be harmful to human beings (1). Several methods have been investigated to reduce ammonia emissions, but due to its high activity at low temperatures, low energy consumption, and ease of use, adsorption has garnered much interest (2).
In this framework, we focus on the synthesis of activated carbon/metal oxide nanoparticles (AC/MO-NPs) using activated carbon prepared from Algerian olive waste. It is important to deposit metals on the carbon surface through impregnation. The deposition of MO-NPs (TiO2 and ZrO2) on the AC must be carried out with special care to ensure intimate contact between the carbon surface and the metal oxides. The final product will be characterized to assess its features.

Once the AC/MO-NPs are successfully prepared, the adsorption capacity of ammonia removal is assessed under dynamic conditions. This procedure involved pre-treating each sample at 120°C for 30 minutes under a flow of N2. Once the reactor has cooled, a flow of ammonia diluted in nitrogen is passed through a fixed bed of activated carbon sample. We were able to study the effect of the type of activating agent, type of MO-NPs, and their loading.

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Keywords: Activated carbon, nanoparticles, adsorption, ammonia removal.

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[*] Speaker

Magneto-Acoustic coupling in Ferrimagnets

Ashwin Kavilen Vythelingum * [1], Laura Thevenard [2], Catherine Gourdon [2], Joao Sampaio [3], Alexandra Mougin [4], Léo Berges [5], Banan Kerdi [3]

[1] Institut des Nanosciences de Paris (INSP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – 4 place Jussieu, 75005 Paris, France
[2] Institut des Nanosciences de Paris (INSP) – Institut des NanoSciences de Paris, CNRS UMR 7588, Sorbonne Université, F-75005 Paris – Sorbonne Université, CNRS, 4 place Jussieu, 75005 Paris, France
[3] Laboratoire de Physique des Solides (LPS) – Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, 91405 Orsay Cedex, France – France
[4] Laboratoire de Physique des Solides – Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, 91405 Orsay Cedex, France – France
[5] Laboratoire de Physique des Solides (LPS) – Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, 91405 Orsay Cedex, France – Université Paris Saclay, France

Ferrimagnets are magnetic materials composed of at least two antiferromagnetically coupled sublattices. The distinct magnetic properties of the latter lifts the two-fold zero-field degeneracy of the magnetic eigenmodes, yielding a "ferromagnetic-like (**FM**)" **mode** and an "antiferromagnetic-like (**AFM**)" **mode**, usually at much higher frequency. The distinct gyromagnetic ratio and moments of the two sub-lattices moreover yield two distinct compensation temperatures: **TMC** and **TAC** where the total magnetisation and total angular momentum vanishes respectively.
The dynamics of these spin-wave (**SW**) eigenmodes have been probed optically, using Brillouin Light Scattering, or pulsed laser excitation, with both experiments relying on fairly inefficient excitation mechanisms. Instead, we propose to rely on the effective field created by a propagating surface acoustic waves (**SAW**), through magnetoelastic coupling, to force precession and induce ferrimagnetic resonance (**SAW-FiMR**). This concept was successful in ferromagnets using gigahertz Rayleigh waves excited piezoelectrically, with the interaction appearing as a strong absorption (decrease) of the wave's amplitude at fields/temperatures satisfying **fSAW=fSW(B,T).**

For this study, we chose the ferrimagnetic alloy Gd30Co70, usually evaporated onto non-piezoelectric substrates. In order to observe SAW-FMR, **we strove to fulfil two conditions**: (i) match SAW and Spin-Wave frequencies, (ii) have a non-zero magneto-acoustic torque. To realise (i), we solved the coupled Landau-Lifshitz-Gilbert equations of Gd and Co sublattices and saw that both AF and FM mode frequencies decrease rapidly with temperature around **TAC** (Inset Fig. 1). In order to further (ii), we generated SAWs along two crystallographic directions which enabled access to two distinct magneto-acoustic torques.
A confirmation of SAW-driven ferromagnetic resonance would open a new road to study the eigenmodes of ferrimagnets. This remote and efficient SAW excitation will allow evaluating magnetic constants, possible modification to the transition temperature and the study of chirality, known to change sign across **TAC**.

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*Speaker

Keywords: Magneto, Acoustic, SAW, FMR, Ferrimagnets, GdCo

Coloration-bleaching mechanisms in nickel-tungsten mixed oxides

Simon Redor * [1,2]

[1] Collège de France - Chaire Chimie du solide et énergie – Chimie du solide et de l'énergie – 11 Place Marcelin Berthelot, 75231 Paris, France
[2] Saint-Gobain Recherche (SGR) – SAINT-GOBAIN – 39, quai Lucien Lefranc, B. P. 135 93303 Aubervilliers Cedex, France

Smart windows can be used in a building to reduce the amount of energy consumed for air conditioning in the summer, and to provide visual comfort to the building's inhabitants. Some of these smart windows are based on electrochromic devices, or "optical batteries": these devices can change color and opacity thanks to electrochemical reactions occurring at two electrodes, a cathodic electrochromic material and an anodic electrochromic material. Although tungsten trioxide (WO3) is often considered the most sensible choice for the cathodic material, the selection of the anodic material is not as clear-cut. In recent years, lithium-nickel-tungsten mixed oxides have proven to be promising candidates to fill the role of anodic material in Li+-based electrochromic devices. However, the nanocomposite structure of these materials, as well as the origins of their electro-optical properties, remain quite nebulous. The goal of this project is to clarify the relationships between the composition, the structure, and the electro-optical properties of LixNiyWzOn materials. To do so, we synthetize monophasic compounds in the Li2O-NiO-WO3 ternary system; they are first prepared as crystallized powders through ceramic syntheses, then as monophasic thin films through a sol-gel spin-coating process. Then, using UV-Visible spectroscopy, Raman spectroscopy, and galvanostatic charge-discharge experiments, we try to draw parallels between the properties of these monophasic compounds and the properties of nanocomposite LixNiyWzOn thin films. In the end, this fundamental knowledge on lithium-nickel-tungsten mixed oxides should lead to the optimization of the electrochromic performances of nanocomposite LixNiyWzOn thin films.

Keywords: Electrochromism, Mixed oxides, Thin films, Li ion, Optics

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*Speaker

Synthesis of La1-

Valentin Grand D'esnon * [1,2], Diana Serrano [1], Simon Delacroix [2],
Sébastien Maron [2], Thierry Gacoin [2], Philippe Goldner [1]

[1] Institut de Recherche de Chimie Paris (IRCP) – Ecole Nationale Supérieure de Chimie de Paris - Chimie ParisTech-PSL, Institut de Chimie du CNRS, Centre National de la Recherche Scientifique : UMR8247, Ministère de la culture, Centre National de la Recherche Scientifique – Chimie ParisTech - PSL, 11 rue Pierre et Marie Curie, 75005 Paris, France

[2] Laboratoire de physique de la matière condensée (LPMC) – Ecole Polytechnique, Centre National de la Recherche Scientifique – Route de Saclay 91128 PALAISEAU CEDEX, France

The exceptional optical properties of rare-earth ion-doped matrices make them ideal candidates for a wide range of applications. Their high optical coherence time makes their use in quantum technologies (quantum memories, quantum telecommunications, qubit, etc.) particularly interesting (1). However, this implies a low luminescence intensity, which can be considerably enhanced by using nanoparticles in optical cavities. These devices amplify the coupling of transitions of interest with light (2). However, coherence time is dependent on the crystalline quality of the materials: size reduction must therefore be accompanied by the preservation of this quality. This is a real challenge.

Here, we present the solid-state synthesis of a lanthanum phosphate matrix doped with europium ions, which has been shown to possess an excellent coherence time. First, the ideal doping ratio to optimize coherence time is determined by photon echo. Secondly, nanoparticles are obtained by pulverizing. Post-synthesis annealing is used to restore crystallinity and coherence time, both of which have been reduced during this stage, and are then studied in detail by Rietveld analysis and photon echo.

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[*] Speaker

Internal coating for nuclear fuel cladding against pellet-cladding interaction (PCI)

Kenza Zougagh * [1]

[1] Service de Recherches en Métallurgie et en procédés Avancés (SRMA) – CEA DES ISAS DRMP SRMA LISL – CEA Saclay, 91191, Gif-sur-Yvette, France

In a nuclear reactor, the cladding of the fuel rod is the subject of particular attention since it constitutes the first safety barrier; its mechanical integrity must therfore be guaranteed in a wide range of conditions, from nominal operation to hypothetical accidental conditions. In this work, we focus on developing an internal thin film coating by DLI-MOCVD process for the nuclear fuel cladding to improve reactors' flexibility and maneuverability to better accommodate power transients.

Keywords: Internal coating, pellet, cladding interaction, DLI MOCVD

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*Speaker

Asymmetric stereodivergent catalysis achieved by means of a switchable asymmetric catalyst built on supramolecular helices

Ran Chen * [1]

[1] Institut Parisien de Chimie Moléculaire (IPCM) – Sorbonne Universités, UPMC, CNRS – France

Despite recent developments on the design of dynamic catalysts, none of them have been exploited for the in-situ control of multiple stereogenic centers in a single molecular scaffold. We report herein that it is possible to select one major amongst four possible stereoisomers of an amino alcohol by means of a switchable asymmetric catalyst built on supramolecular helices. Hydrogen-bonded assemblies between a benzene-1,3,5-tricarboxamide (BTA) achiral phosphine ligand coordinated to copper and an enantiopure BTA monomer are engaged in a concomitant copper-hydride catalyzed hydrosilylation and hydroamination process, yielding mainly one of the possible stereoisomers in good yield. The nature of the product stereoisomer is related to the handedness of the helices and can thus be directed in a predictable way by the nature of the major enantiopure BTA present in the assemblies. Accordingly, a sequential reaction, during which the handedness of the supramolecular helices is switched in between the hydrosilylation and hydroamination steps, mainly yields the diastereoisomer that cannot be obtained in the aforementioned concomitant process. The strategy allows all stereoisomers to be obtained with similar selectivities. This work paves the way for the development of supramolecular helical catalysts as a platform to readily access molecules embedding several stereogenic centers.

Keywords: Supramolecular catalysis, Chirality amplification, Stereodivergent synthesis

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*Speaker

Implementing different supramolecular helical platforms for asymmetric catalysis

Antoine Perennes * [1], Matthieu Raynal† [1]

[1] Institut Parisien de Chimie Moléculaire (IPCM) – Chimie Moléculaire de Paris Centre, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – France

Chirality has raised a great awareness for the research community which has widely developed enantiopure chemicals, including biologically active drugs, chiral catalysts, homochiral materials, etc.Small molecules must contain a stereogenic center, an axis or a plane of chirality to be considered as chiral, while the macromolecules may have an inherently chiral structure due to the self-organization of their molecular units into helices. Supramolecular helical polymers, generated by of self-association of monomers by means of weak interactions (hydrogen bonding, π-π stacking, and so on), are particularly attractive. Preparing supramolecular polymers featuring a defined handedness may be challenging. There are various ways to obtain homochiral (i.e. single handed) helices but the most common concept relies on the "sergeants-and-soldiers" (S&S) effect. It consists of mixing enantiopure molecules, called the sergeants, and achiral monomers as the soldiers. The presence of a little amount of sergeants is sufficient to dictate a single sense of rotation to the corresponding helices. Triarylamine trisamides (TATAs) forming supramolecular polymers by hydrogen bonding has been deeply studied for its electronic and spintronic properties. They possess a great ability to exhibit particularly powerful chirality induction and amplification effects. In addition, it has been demonstrated that the handedness of helical assemblies formed by enantiopure TATA monomers can be switched with the temperature and inverted according to assembly being on kinetic or thermodynamic control.We are now interesting in preparing TATA monomers for the development of supramolecular helical catalysts, investigating the corresponding S&S-type mixtures in various analytical techniques (Circular Dichroism, Fourier-Transformed InfraRed) and applying them in a copper-catalyzed hydrosilylation process.

Keywords: Supramolecular chemistry, Polymers, Catalysis

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*Speaker

†Corresponding author: matthieu.raynal@sorbonne-universite.fr

Self-assembling, narrow-bandgap rylenes for photovoltaic applications

Simon Peyras * [1]

[1] Institut Parisien de Chimie Moléculaire (IPCM) – Chimie Moléculaire de Paris Centre, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR8232 – Sorbonne-Université, 4 place Jussieu 75252 Paris Cedex 05 BÃćtiment F/74, France

Rylenes are a family of aromatic molecules that are widely used in organic photovoltaic (OPVs) devices due to their chemical, thermal stability, anf their capacity for electron transport (1). They are good Acceptors, and they can be linked covalently to Donors, which permits the control of the properties of the active layer. These push-pull type rylene derivatives can be exploited as small molecule or polymer-based dyes in the active layer of the solar cell (2)
But they can also be arranged molecularly, and supramolecularly in the solid state (3). This self assembling process helps the material to have better properties.
Rylene derivatives, and especially perylene diimide derivatives, are known to strongly aggregate via π-π stacking, which quenches energy conversion in OPVs. To overcome this, strategies concerning the structure of the PDI core lead to developping interesting functional assemblies (columnar, straight or rotational packing). (3)

By studying and understanding the relationship between supramolecular arrangement and the electronic properties of rylene-based self-assembling nanostructures we will be able to advance the engineering of more complex, functional nanomaterials.

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Keywords: organic synthesis, organic photovoltaic, self assembly, liquid crystals

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[*] Speaker

Synthesis of Janus Nanocylinders for Surface Patterning

Mingsheng Ji * [1], David Siefker [1], Sandrine Pensec [1], Jutta Rieger [1], Laurent Bouteiller† [1]

[1] Sorbonne Université – Sorbonne Université UPMC Paris VI – France

Janus nanorods (or Janus nanocylinders) are one-dimensional colloids that have two faces with different compositions and functionalities, and are useful as building blocks for advanced functional materials. Recently in our group, we have developed a chain transfer agent (CTA) with hydrogen bonding to synthesize polymers via reversible addition–fragmentation chain transfer (RAFT) polymerization. Herein, we use this versatile strategy to synthesize various _8_4_ polymers. By co-assembly with _4_8_PDMAc, a library of Janus nanorods should be obtained. The Janus nanorods will then be transferred onto silicon substrate for surface patterning applications.

Keywords: Janus nanorods, RAFT polymerization, Coassembly.

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*Speaker

†Corresponding author: laurent.bouteiller@upmc.fr

Silicon-delivering cellularized biomaterials for dental repair

Daline Mbitta Akoa [*] [1]

[1] Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Institut de Chimie du CNRS,
Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne Université, 4 place
Jussieu, 75252 Paris Cedex 05, France

Silicon (Si) is a trace element that is known to be beneficial for normal bone formation. Positive effects of Si from the diet as well as from Si-containing biomaterials, such as bioactive glasses, have been demonstrated in bone repair (1). Besides, these Si-based materials are also widely used for dental repair (2), although the issue of silicon's effect on dental cells has not received adequate attention so far. In this context, the present project aims at preparing materials that would allow the study of the role of silicon on dental tissue formation.

The current results focus on the *in vitro* effects of ortho-silicic acid on the viability, differentiation, and mineralization of human dental pulp stem cells (hDPSCs). The hDPSCs encapsulated in plastically compressed dense collagen hydrogels were grown in a mineralizing induction medium supplemented with Si(OH)4 at concentrations of 0, 10 and 100 μM for 24 days. No cytotoxic effects at 10-100 μM of Si(OH)4 were observed in the cells. Si(OH)4 at physiological concentrations (10μM) allowed matrix mineralisation and collagen matrix remodelling, while supraphysiological reduced mineral formation *in vitro*. Ongoing research on Si(OH)4-releasing biomaterials will provide further insights.

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Keywords: Silicic acid, Human dental pulp stem cells, Plastically compressed dense collagen hydrogel

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[*] Speaker

Mechanistic insights into elastomer frictional wear using damage-reporting mechanophores

Ombeline Taisne * [1], Jean Comtet [2], Costantino Creton [2]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France
[2] SIMM laboratory, ESPCI – CNRS : UMR7615 – France

Tire wear due to friction is a major issue for tire manufacturers. During wear by fatigue of tyre tread materials (1)(2), the material at the surface of the tyre tread undergoes slippage at the road-tyre interface each time the wheel turns, leading ultimately to erosion through mass loss and wear. However, a mechanistic understanding of elastomer wear by fatigue is still incomplete, due to the difficulty in accessing the local damage field at the surface of the material. Here, we take advantage of recently developed mechanophore molecules (3)(4) to characterize molecular damage gradients in the sub-surface. Once chemically incorporated in known quantities in the elastomer network as cross-linkers, these molecules can be used to spatially probe molecular scission events damaging the integrity of the network (5). Specifically, we use this detection strategy to characterize and quantify the damage gradient at a molecular scale in multiple interpenetrated networks elastomers made of poly (ethyl acrylate). Following mild friction cycles of the elastomer material against glass, we uncover that damage extends under the surface of the elastomer over tens of micrometers and suggest a 2-step damage mechanism of damage accumulation in the sub-surface, followed by erosion of the material. We further probe the impact of network pre-stretch, normal pressure and glass roughness on both wear rates and subsurface damage. Thanks to a new cross-linking synthesis in soft conditions, and a versatile method of infusion of the mechanophore in the network, we were then able to incorporate the mechanophore as a cross-linker inside a readily vulcanised, silica-filled, SBR matrix. In addition to providing a new tool for the spatial quantification of chain damaging events, it is the first time that the sub-surface damage gradient due to frictional wear is measured experimentally in these industrially relevant materials.

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[*] Speaker

A Guanidium Salt as a Chaotropic Agent for Aqueous Battery Electrolytes

John Brown * [1]

[1] John Brown (Chimie du Solide et de l'Energie (CSE)) – Chimie du Solide et de l'Energie - Collège de France – Collège de France, UMR 8260, 75231 Paris Cedex 05, France, France

Aqueous battery electrolytes face limitations due to water's narrow electrochemical stability window (ESW) of 1.23 V. To address this issue, water-in-salt electrolytes (WISE) were proposed, using highly concentrated lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salts to expand the ESW beyond 3 V (1). The high concentration of anions promotes the formation of passivating layer on the negative electrode restricting the hydrogen evolution reaction (HER), while forming a hydrophobic layer on the positive electrode mitigating the oxygen evolution reaction (OER). However, WISE have not completely resolved the problem, as the HER remains an issue during cycling and rest periods (2). Recent studies have tackled this persistent HER problem by introducing additives to WISE such as urea, which disrupts the hydrogen bonding network (HBN) of water, reducing water reactivity (3). Interestingly, the Hofmeister series, which characterizes ion interactions with the HBN of water, suggests that Li+ cations are kosmotropic, hence strengthening HBN. Thus, an interesting avenue is combining TFSI with chaotropic cations, like guanidium (Gdm), which could benefit from the characteristics of TFSI while harnessing similar effects to urea. Although GdmTFSI has been synthesized previously, it lacks comprehensive characterization (4). This work presents a synthesis procedure for GdmTFSI, crystal structure determination, and detailed chemical analysis. Aqueous solutions of the salt were investigated using IR and viscosity measurements, revealing that the Gdm cation disrupts the HBN, expanding the ESW (5). Further research is needed to explore its compatibility with Li-based salts, offering potential solutions to enhance electrolyte performance.

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Keywords: Batteries, Aqueous electrolytes, Hofmeister series

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*Speaker

Biomineral pigmentation in the Paracentrotus lividus sea urchins

Claudio Ferreira * [1], Nadine Nassif [1], Marie Albéric† [1]

[1] Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne Université, 4 place Jussieu, 75252 Paris Cedex 05, France

The wide range of colors observed in sea urchins is related to the incorporation of organic pigments within their biominerals, especially their spines (1, 2, 3). Pigments are poly-hydroxylated naphthoquinone molecules (PHNQs) that are produced within the so-called red spherule cells (RSCs) taking part into the immune system of the urchins (4, 5, 6). The mechanisms by which PHNQ molecules are biosynthesized and later released to be incorporated into the biomineral are not yet fully understood. Our aim is to better understand such processes in Paracentrotus lividus sea urchins, which commonly display green and purple colors. By using HR-MS and liquid-state 1H NMR, we observe that Spinochrome A is the main PHNQ molecule although extracted from the two different colored spines. Further, SDS-PAGE analyses of the organic biomolecules extracted from spines along with pigment molecules reveal the presence of PHNQ-complexes. Remarkably, we evidence the presence of a green macromolecule that is exclusive to green spines, thus likely playing an important role in color determination. FTIR spectra of the different organic fractions confirm the protein signatures and show the presence of polysaccharides and lipids as well. TEM micrographs of RSC at the vicinity of growing mineral reveal the presence of pigment vesicles undergoing maturation prior to pigment release. In addition, we identify a polysaccharide layer that internally coat and possibly stabilize these vesicles (e.g. against acidic pH). Finally, in vitro crystallization assays, performed with spine organic extracts as additives, indicate an influence of over calcite formation, with extracts from green spines having a stronger effect over crystal shape, possibly due to differences in organic content, particularly its exclusive chromo-macromolecule. Our observations suggest that pigmentation and biomineralization in sea urchins are mutually related processes, through a pathway that is certainly quite intricate.

Keywords: polyhydroxylated naphthoquinones, pigmentation, biomineralization

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[*] Speaker

[†] Corresponding author: Marie.alberic@sorbonne-universite.fr

Multiscale probing of an unusual structural transition in chiral and functional BTA helical assemblies

Huanjun Kong * [1], Matthieu Raynal† [1]

[1] Institut Parisien de Chimie Moléculaire – Sorbonne Universités, UPMC Univ Paris 06 CNRS Institut Parisien de Chimie Moléculaire, UMR 8232 Chimie des Polymères – France

Benzene 1,3,5-tricarboxamides (BTAs) comprise three amides attached to a benzene core.(1) It generates supramolecular helical rods through a combination of threefold H-bonds and π-π stacking interactions. The dynamic properties of BTA supramolecular polymers make it necessary to use multifarious analytical techniques to get a multi-scale structure of their assemblies.(2) Due to cooperative effects, subtle structural transition in between different types of supramolecular assemblies can be detected for BTA and BTA-related supramolecular polymers.(ref: Meijer for water-containing BTA assemblies)(3) However, a direct relation between the nature of this transition at the molecule level and the related properties at the macromolecular scale is rarely established. Supramolecular polymers of BTAPPh2*(S),(S)* (Figure 1a) were characterized by Fourier-Transform Infrared (FT-IR), Variable-Temperature Fourier-Transform Infrared (VT-FTIR, Figure 1b), Circular Dichroism (CD) and Variable-Temperature Circular Dichroism (VT-CD, Figure 1c) analyses as well as SAXS and SANS analyses. All these data indicate that an intramolecular structural transition occurs in the supramolecular helices in a relatively narrow range of temperature. This structural transition influences both the rheological and catalytic properties of the supramolecular assemblies. This transition was probed by MM/MD calculations to try to determine the nature of the conformational change at the origin of the structural transition at the molecular level.

Keywords: BTA supramolecular polymers, helical assemblies, structural transition

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*Speaker

†Corresponding author: matthieu.raynal@sorbonne-universite.fr

Boron phosphide nanocrystals : Synthesis, structure, reactivity and properties

Amandine Séné * [1], David Portehault [2], Capucine Sassoye [3], Christel Gervais Stary [3]

[1] Sorbonne Université, CNRS, Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Sorbonne Université, CNRS, Sorbonne Université, CNRS : UMR7574 – France
[2] Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – CNRS : UMR7574 – France
[3] Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Sorbonne Universités, UPMC, CNRS – France

Boron phosphides exhibit exciting properties, from hardness to photoelectrocatalytic properties. Cubic boron phosphide (c-BP) is especially a good candidate for photocatalytic water splitting1–3 and CO2 reduction4. On the other hand, bulk c-BP is well known to be a hard material5. Such properties would benefit from nanostructuration.

The synthesis of nanostructured c-BP is challenging, its framework of covalent bonds requires a high energetic cost hence only one synthesis has been reported to provide c-BP nanoparticles6. This synthesis results in contaminated particles and uses harmful reagents such as HF.

I have developed a new bottom-up synthesis of c-BP crystalline nanoparticles with an average diameter of 5 nm, via molten salt media to hasten reactions7, even below the temperature usually employed to reach this compound thus delivering new nanomaterial with high surface area.

During this poster session, this brand new synthesis will be presented along with structural and morphological features of these nanocrystals. Their properties as photoelectrocatalysts and reactivity with transition metals in molten salt and under high pressure (3 GPa) salt will be presented as well.

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Keywords: boron phosphide, nano, catalyst, hard, material, molten salt, synthesis, high pressure

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*Speaker

Development of microlasers based on semiconductor nanocrystals in a polymeric microcavity

Charlie Kersuzan * [1,2]

[1] Nanostructures et optique – Institut des Nanosciences de Paris – France
[2] Laboratoire de Physique et d'Etude des Matériaux (UMR 8213) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – France

The development of microlasers and more generally of microcavities has been widely developed in the last decades. Microcavities allow to obtain an important optical confinement and a strong light-matter interaction. These microlasers can be used as light sources integrated in photonic circuits, but also as biological detection systems. We use semiconductor nanocrystals (scNCs) as gain media, because they possess interesting optical properties: stable emission and control of the emission wavelength over the entire visible and near infrared range. Recent works have also shown the efficiency of scNCs as gain media with low stimulated emission thresholds. We present the realization of optical microcavities containing scNCs. First, we solubilize scNCs in a negative photoresist to obtain a homogeneous distribution, then we fabricate pillar-shaped optical cavities in this resin by photolithography. Finally, a spectroscopic characterization of the optical properties of scNCs in these micropillars is performed, highlighting the emitter-cavity coupling.

Keywords: microlaser, whispering gallery modes, quantum dots, microcavity, photonic, nanocrystals

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*Speaker

Novel TADF Molecular Materials for High Performance Light Emitting Diodes based on cyclophane cores

Chao Wu * [1]

[1] Institut Parisien de Chimie Moléculaire (IPCM) – Chimie Moléculaire de Paris Centre, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR8232 – Sorbonne-Université, 4 place Jussieu 75252 Paris Cedex 05 BÃćtiment F/74, France

As the third generation of Organic Light Emitting Diode (OLED), thermally activated delayed fluorescence (TADF) emitters can achieve 100% internal quantum efficiency without using precious metals and thus provide excellent device performances. This project aims at designing and synthesizing a series of new organic TADF light emitting compounds based on cyclophane cores functionalized with donor and acceptor units. These three-dimensional luminescent derivatives present a rigid structure with a small distance between the D and A, leading to strong through space D-A interactions and charge transfer (CT) states. These architectures show low triplet energy gaps (ΔEST) and good photophysical properties such as photoluminescence quantum yields (PLQY) up to 82% in Toluene. In addition, OLED devices based on these materials as emitting layer display good performances with a maximum external quantum efficiency (EQE) about 12%.

Keywords: OLED, TADF, Cyclophane cores

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*Speaker

Impact of the surface chemistry of 2D nanoplatelets on cation exchange

Lina Makke * [1]

[1] Laboratoire de Physique et d'Etude des Matériaux (UMR 8213) (LPEM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin, 75231 Paris cedex 05, France

Among nanocrystals, 2D zinc blende nanoplatelets (NPLs) provide the highest level of growth control, resulting in sub-monolayer roughness on their surface and hence on their thickness. This characteristic enables a uniquely narrow spectral linewidth. The synthesis of 2D particles is now well controlled with cadmium chalcogenides but the growth process remains difficult to extend to other materials. Therefore, an alternative strategy to achieve a roughness-free 2D object is to perform cation exchange on as-synthesized NPLs. Nevertheless, if not properly conducted, this strategy leads to dramatic shape reconstruction, resulting in the loss of beneficial properties. As part of my thesis, I demonstrated that **surface chemistry** can significantly impact the kinetic and thermodynamic properties of the cation exchange process. When performing copper exchange on CdSe NPLs, I found that thiols are the most suitable ligands for shape preservation. This can be attributed to the ligand-induced lattice contraction on CdSe, which minimizes lattice distortion during cation exchange. Conversely, I determined that the initial flatness of the particle, ligand length, and ligand binding strength are not critical for maintaining the shape, although they impact the reaction duration.

Keywords: cation exchange, surface chemistry

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*Speaker

Oscillatory fracture paths in the cutting of elastomer sheets

Svetlana Glukhova * [1,2], Matteo Ciccotti [3], Frédéric Lechenault [4]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France
[2] Laboratoire de physique de l'ENS - ENS Paris – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Université Paris Cité, Département de Physique de l'ENS-PSL – France
[3] Sciences et Ingénierie de la Matière Molle (UMR 7615) (SIMM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin 75231 PARIS CEDEX 05, France
[4] Laboratoire de physique de l'ENS - ENS Paris (LPENS) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Université Paris Cité, Département de Physique de l'ENS-PSL – 24, rue Lhomond75005 Paris, France

Cutting is a ubiquitous process with wide ranging implications. Our strategy is to deliberately select experimental conditions where cutting soft materials indeed leads to the generation of large shape changes in the cut parts in order to develop an appropriate modelling that combines nonlinearities due to large geometry changes during the cutting and those coming from the nonlinear material response under large strains. Moreover, this morphogenetic investigation can lead to smart techniques to produce complex shapes starting from simple tools(1). Elastic rubbers are good candidates for this first investigation since they allow large strain with a well-defined nonlinear response.

In this work, we investigate a spontaneous oscillatory pattern that originates when cutting an elastomer sheet under an imposed prestretch (pure shear sample(2)) and imposing a constant velocity to the blade. The advantage of this configuration is that the applied stretch allows the blade to set free from most macroscopic friction acting on its sides, and to allow for fracture propagation in similar conditions without a blade in the same soft material.

We obtained the occurrence of two novel instabilities that perturb the cutting process and give rise to regular morphologies on the fracture surfaces. The first instability occurs in most conditions and it gives rise to a very regular sinusoidal oscillation in the fracture surfaces. The second instability occurs when using blunter blades with a weak pre-stretch and it causes larger out of plane motions of the sample during the cutting due to some buckling wrinkles. We investigated the dependency of these two instabilities for a series of elastomers with variable modulus, and changing the applied stretch, the blade sharpness angle, the cutting velocity with the aim of developing a consistent modelling of the final shape of the cut surfaces.

Keywords: Cutting, fracture mechanics, oscillations

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*Speaker

Quasi-harmonic approximation breakdown: consequences on the thermal transport at extreme condition of Earth's lower mantle

Chabane Saadi [*] [1]

[1] IMPMC$_{T}horiequantiquedesmatriaux -$
$-Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie - -France$

MgO is a material important for many technological applications as well as in planetary sciences since it is an archetypal mineral comprising the Earth's lower mantle (LM). Here, we address how the anharmonic effects, due to phonon scatterings, influence phonons' energies and lifetime at the extreme high-temperature high-pressure conditions pertinent to the LM (pressure between 24 and 135GPan temperatures up to 3000K) and their consequences on the lattice thermal conductivity. Where our previous work highlighted the importance of anharmonicity on the lattice dynamics of MgO at ambient conditions, at high-pressure but ambient temperature, and at high temperatures but ambient pressure (1,2), the simultaneous effects of the high-pressure and high temperature were not addressed yet.
In this presentation, I will present the results of ab-initio calculations of the phonon anharmonicity in two cases: I) ambient pressure and high temperature up to T=1223K, covering the range where calculations can be compared to existing experimental results ii) at Earth's lower mantle conditions with T-P in the range from 1900K-24GPa to 3000K-130GPa. High-temperature effects on the phonon energies and linewidths due to the 3 and 4 phonons scatterings are considered in the framework of perturbation theory. These results are compared with Infrared spectroscopy and Inelastic x-ray scattering measurements carried out by our group. The high-temperature case permits benchmarking the joint DFPT (3) and SSCHA (4) approach in describing the anharmonic lattice dynamics of MgO. Once validated against the experiments, calculations are extended to the lower mantle conditions to discuss the effect of pressure and temperature on the anharmonicity of MgO. Finally, I will show the consequences of the anharmonic terms on the lattice thermal conductivity of MgO at LM conditions in relation to phonons scattering.

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[*] Speaker

Abstract_62RoselliBaptiste

Baptiste Roselli * [1]

[1] De la Molécule aux Nanos-objets : Réactivité, Interactions et Spectroscopies (MONARIS) – Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne-Université BÃćtiment F 4, place Jussieu - 75252 PARIS Cedex 05, France

Abstract poster 62 JED 397 2023

Keywords: Abstract poster 62 JED 397 2023

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[*] Speaker

Iron Oxides under extreme pressure and temperature condition for planetary interiors

Juan Pintor * [1], Marion Harmand [2], Delphine Cabaret [3]

[1] Minéralogie, Pétrologie et physique planétaire / Théorie quantique des matériaux[IMPMC]
(IMPMC$_MP3) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$
[2] Minéralogie, Pétrologie et physique planétaire [IMPMC]
(IMPMC$_MP3) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$
[3] Théorie quantique des matériaux [IMPMC]
(IMPMC$_TQM) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$

The study of the atomic and electronic structures of the different phases of iron oxides is of considerable importance for planetary interiors. Indeed, iron and oxygen are two of the most abundant elements found in telluric planets. Iron oxides play a major role in the mineralogy of the mantle and core of Earth- and Super-Earth-type exoplanets.

My study is being conducted along two lines: 1) The use of ab initio simulations to simulate crystalline structures at high pressures and obtain the corresponding X-ray absorption spectra and diffractometers. 2) The use of dynamic laser compression combined with ultra-fast X-rays produced by free-electron lasers (EuXFEL in Germany, LCLS in the USA, SACLA in Japan, etc.). This approach enables in-situ observation of phases and electronic properties at high pressure.

For this presentation I will focus on our last experiment, during which we performed ultra-fast time-resolved X-ray Absorption Near Edge Spectroscopy (XANES) measurements on laser-compressed Fe2O3 at the High Power Laser Facility (HPLF) of ESRF-ID24 beamline. Our XANES data provide information on time-resolved structural transformations by showing changes in the pre-edge, the white line and the 1 st Extended X-Ray Absorption Fine Structure (EXAFS) oscillation within hundreds of ps after the shock breakout from the samples. More severe spectral changes are observed at longer delays between the X-ray probe and the shock, during its thermodynamic release. We will present a detailed time-resolved study of the XANES changes as a function of pressure and temperature, along the Fe2O3 Hugoniot thermodynamic path and release.

Keywords: iron oxides, phase diagram, phase transition, dynamic compression, laser shock compression, X, ray absorption

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[*] Speaker

Mechanics of solid polymers: Understanding and modelling the creep response

Martin Roman-Faure * [1], Hélène Montes [1], FranÃğois Lequeux [1], Antoine Chateauminois [1]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France

The structure of amorphous polymers is disordered and as a consequence they exhibit macroscopic properties that corresponds to complex averages of the local ones. Modeling and understanding the mechanics of amorphous polymers remains a challenge. In this work we focus on weak non-linearity under creep and show that they reveal stress heterogeneities.

Indeed, it has been recognized since two decades, that amorphous polymers exhibit nanoscale dynamical heterogeneities. The associated relaxation time distribution varies by orders of magnitudes. For a typical homopolymer, the time distribution spans over more than 4 decades. A glassy polymer can thus be considered as a material paved with nanoscale domains having their own relaxation time (*Ediger, et al. Annu. Rev. Phys. Chem. 2000*).

In creep, nonlinearity is observed, characterized by an acceleration of the strain time evolution as compared to the linear one. The observed ratio in time to reach a given compliance value is defined as the creep acceleration function. Different models exist to describe the behavior of acceleration fucntion. The experimental determination of the local acceleration function is tricky. Using a poly(etherimide) (PEI) amorphous polymer as a model system, we show that in a weakly nonlinear creep regime, the nonlinear response is similar at the macro scale to and at the local scale for small values of strain. However, for increasing creep strains a difference is observed between the local law and the macroscopic one. We suggest that this difference is due to the amplification of local stress in unrelaxed domains. Within this framework, it is possible to determine from the creep response, the ratio of the local stress in stress bearing domains to the applied macroscopic stress. As a conclusion, creep acceleration measurements reveal the stress heterogeneities in amorphous polymers.

Keywords: amorphous polymers, glassy polymers, nonlinear mechanics

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[*] Speaker

Damaging polyamide 6,6 with road salts

Edwige Lay * [1,2], Annie Colin [1]

[1] Matériaux Innovants pour l'Energie – Chimie-Biologie-Innovation (UMR 8231), ESPCI Paris, PSL Research University – France
[2] Technocentre Renault [Guyancourt] – Renault – France

Polyamide 6,6 (PA6,6) is a well-known and widely used polymer in the automotive industry. During its lifetime, it may come into contact with road salts such as NaCl, MgCl2 or CaCl2. In the literature, authors report an environmental stress cracking (ESC) behavior due to the exposure to some of these saline solutions. However, to the best of our knowledge, there is no consensus on the absorption and cracking mechanisms of ESC.
Without applied stress, during immersion tests, the resulting mechanical effects (plasticization) have been related to the water activity in the saline solution. SEM-EDX and μXRF measurements have been carried out to quantify the absorbed ions, which are present but not significantly enough to affect the tensile behavior.

In the presence of a constant tensile stress, when the contact with a droplet of road salt solutions occurs, different cracking behaviors have been demonstrated. At room temperature, no cracking is observed at stresses lower than the yield stress. At the yield stress and in dry samples:

- water induces local plasticization wrinkles but the diffusion path has yet to be observed

- NaCl-type salts create thin crazes with no detected absorption of salts

- CaCl2-type salts create large crazes with detected absorption of salts

The distinction between the different behaviors is related to the localization of plasticity and the plasticity instabilities created by the saline solutions.
Further experiments will be carried out to describe these instabilities by considering various hypotheses: surface tension effects, chemistry, osmotic pressure in the crazes, ...

Keywords: Polyamide 66, deicing salts, environmental stress cracking

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*Speaker

Copper silicophosphides: new ternary nanocrystals as electrocatalysts for carbon monoxide reduction

Anissa Ghoridi * [1], Ngoc Huan Tran [2], Carlos Victor Mendonca Inocencio [1], Séné Amandine [1], Baron Marzena [1], Daniel Janisch [1], Edouard De Rolland Dalon [1], Fernando Igoa [1], Emile Defoy [1], Antoine Miche [1], Christel Gervais Stary [1], Cristina Coelho-Diogo [1], Pierre-Olivier Autran [3], Andrea Zitolo [4], Isabelle Génois [1], Sandra Casale [1], Marc Fontecave [2], David Portehault [1]

[1] Sorbonne université - Faculté des Sciences et Ingénierie (SU FSI) – Sorbonne Université - CNRS – 4 place Jussieu 75005 Paris, France
[2] Collège de France – Sorbonne Université - CNRS - Collège de France – France
[3] Synchrotron SOLEIL (SSOLEIL) – Centre National de la Recherche Scientifique – L'Orme des Merisiers Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX, France
[4] European Synchroton Radiation Facility [Grenoble] (ESRF) – European Synchrotron Radiation Facility (ESRF) – 71, avenue des Martyrs, CS 40220, 38043 Grenoble Cedex 9, France

Incorporating p-block elements into transition metals offers a mean to fine-tune their electrocatalytic properties through localized structural distortion, charge transfer, and hybridization (1). Beyond simply doping, the design of compounds with specific compositions and crystal structures can significantly expand the range of accessible properties. Notably, copper phosphides and silicides have been explored for their efficiency as catalysts or pre-catalysts in electrochemical water splitting (2) and as anodes in Li-ion batteries (3,4). However, the properties of ternary copper silicophosphides, which possess unique structures distinct from binary phases, have been little investigated. Currently, only three ternary copper phases are known (CuSi2P3, CuSi4P3, Cu4SiP8) (5,6), and have remained at the status of scientific oddities.

To boost catalytic activity and selectivity for the generation of high-value added products containing C-C bonds in the electrocatalysis of the CO2 reduction reaction (CO2RR) and of the CO reduction reaction (CORR), one approach is to create single metal active sites, which can deeply modify catalytic cycles compared to metal clusters or nanoparticles (7,8). However, maintaining these single atom sites in an isolated state during electrocatalysis poses a significant challenge. Our strategy focuses on stabilizing these sites within crystallographic structures by seeking additional stabilization through the promotion of covalent bonding to establish a rigid crystal structure. It is also imperative to design nanostructures with a high surface-to-volume ratio, thereby amplifying catalytic activity. Copper silicophosphides present an ideal candidate for this purpose.

Here, we introduce the synthesis of copper silicophosphide CuSi2P3 nanocrystals using molten salts to initiate nanoparticle formation and control growth (9). In-situ X-ray diffraction measurements at ESRF ID11 synchrotron beamline during synthesis reveal crystallization mechanism. After extensive nanomaterial characterization (structure, composition, morphology: TEM, HRTEM, STEM-EDX, EDS mapping, XPS), we explore CuSi2P3's promising electrocatalytic

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*Speaker

properties for CORR using in-situ X-ray absorption spectroscopy at SOLEIL SAMBA synchrotron beamline.

Keywords: copper ternary compounds, nanocrystals, molten salts, CO reduction reaction

Synthesis and characterization of narrow bandgap II-VI semiconductor 2D nanoparticles

Ningyuan Fu * [1]

[1] Ningyuan FU – ESPCI-LPEM – France

Semiconductor nanoparticles have optical properties tunable to their size and composition. Among these particles, 2D nanoplatelets (NPLs), are promising materials thanks to their optical properties devoid of inhomogeneous broadening. However, the optical properties are limited to the visible range when working with cadmium chalcogenides. To reach the infrared range, narrower band gap semiconductors need to be considered, such as mercury chalcogenides. The goal of the project is to push further the optical properties in the IR range while keeping a narrow emission. However, the direct synthesis of mercury chalcogenide NPLs is thermodynamically unfavored, and the current cation exchange method is limited to 3 exchanged atomic plans from cadmium chalcogenide to mercury chalcogenide. A new cation exchange approach is developed by using silver cation as the catalyst to boost the cation exchange between mercury cation and cadmium chalcogenide NPLs. Different cation exchange conditions are investigated in order to get NPLs with better morphology and optical properties. Finally, a series of NPLs with tunable emission in NIR are obtained.

Keywords: Semiconductor, Nanoplatelet, Infrared

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*Speaker

A Quantitative Approach to Study the Adhesion Force of Microalgal Cells

Paula Araujo Gomes * [1,2], Jean-Baptiste D'espinose [3], Tassiane Astuti [3], Nicolas Desprat [4], RaphaÃńl Jeanneret [4], Bruno Lartige [5], Valérie Molinier [6], Emilie Verneuil [7], Nicolas Sanson [8]

[1] SIMM ESPCI – SIMM, ESPCI Paris, Université PSL, Sorbonne Université, CNRS – France
[2] TotalEnergies OneTech – TotalEnergies OneTech, PÃťle dâĂŹEtudes et Recherche de Lacq – France
[3] SIMM/ESPCI – ESPCI Paris, PSL Research University – France
[4] lpens – LPENS – France
[5] GET – Géosciences Environnement Toulouse (GET) âĂŞ Observatoire Midi-Pyrénées, Université Paul Sabatier [UPS] - Toulouse III, CNRS: UMR5563 – France
[6] TotalEnergies OneTech – TotalEnergies OneTech – France
[7] SIMM ESPCI – CNRS : UMR7615 – France
[8] SIMM ESPCI – Université Pierre et Marie Curie - Paris 6 – France

The surface interactions between unicellular microorganisms regulate their colloidal stability in an aqueous medium. Therefore, an accurate description of the adhesion forces between microalgal cells is critical to understanding how microalgae concentrations can change in their biotope or during harvesting processes. We report the adhesion between two microalgal cells under water using the dual micropipette assay. In this technique, two microalgal cells held at the end of micropipettes are brought into contact. The dynamics of the adhesion force is obtained by pulling the cells apart; therefore, the adhesion is quantitatively characterized under varying biological conditions. The results were compared with sedimentation tests under similar conditions. This is a step towards better understanding the not well-known mechanism of interactions between microalgal cells.

Keywords: Microalgae, Flocculation, Adhesion

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*Speaker

Hydrogel membranes for a selective filtration

Sixtine De Chateauneuf * [1,2], Cecile Monteux [3], Bruno Bresson [3], Sabrina Belbekhouche [4]

[1] Sciences et Ingénierie de la Matière Molle (UMR 7615) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7615 – France
[2] Institut de Chimie et des Matériaux Paris-Est – Institut de Chimie du CNRS, Université Paris-Est Créteil Val-de-Marne - Paris 12, Centre National de la Recherche Scientifique – France
[3] Sciences et Ingénierie de la Matière Molle (UMR 7615) (SIMM) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – ESPCI, 10 rue Vauquelin 75231 PARIS CEDEX 05, France
[4] Institut de Chimie et des Matériaux Paris-Est (ICMPE) – Institut de Chimie du CNRS, Université Paris-Est Créteil Val-de-Marne - Paris 12, Centre National de la Recherche Scientifique – 2-8, rue Henri Dunant 94320 Thiais, France

Hydrogels are networks of polymer molecules bound together by covalent bonds. While the diffusive transport of molecules in hydrogels has been well studied in the context of drug delivery, the hydrodynamic transport of water, molecules, and particles in hydrogels in the context of filtration has been barely studied.

Recently our group has synthesized macroporous hydrogels based on the UV cross-linking of polyethylene glycol diacrylate (PEGDA) in water, a mechanically resistant hydrogel. To control the permeability of PEGDA hydrogels we showed that crosslinking PEGDA in the presence of free polyethylene glycol (PEG) chains dramatically increases water permeability by several orders of magnitude. We found that these PEG chains do remain trapped in the matrix and provide nanometric defects that control the permeation of nanoparticles.

In this work, our goal is to use the fact that these free chains remain trapped in the matrix to functionalize the hydrogels. Hence we replace the free PEG chains with electrostatically charged polymers like polyacrylate (PAA). This allows us to obtain selective membranes able of adsorbing or repulsing solutes. As a proof of concept, we chose to filter a positively charged dye (Methylene Blue) and a zwitterionic one (Rhodamine B). This selectivity can be reversed by protonation of the PAA due to an acidification of the pH. Furthermore, we designed a similar membrane capable of making hydrogen bonds with a small acidic molecule to retain it.

This approach will allow the design of new hydrogels for water treatment or the separation of molecules of pharmaceutical interest.

Keywords: hydrogels, membrane, filtration, selectivity

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*Speaker

Rediscovering tempera grassa: physicochemical properties of emulsion-based paints

CÃťme Thillaye Du Boullay [*,†] [1], Laurence De Viguerie [1], Maguy Jaber [1]

[1] Laboratoire d'Archéologie Moléculaire et Structurale (LAMS) – Université Pierre et Marie Curie - Paris 6, Institut de Chimie du CNRS, Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – UPMC 4 Place Jussieu 75252 Paris Cedex 5, France

Painting technique in Europe went through a major shift in the 15th century, thanks to the newly-developed control of the drying of oil. The use of egg yolk as a binder in *tempera* paintings was gradually replaced by oil paint. This transitional period probably saw the occasional use of mixed techniques, in which both types of binders, egg and oil, are present in a painting, sometimes even mixed together in a single layer of paint, a technique called *tempera grassa* (1). The description of the macroscopic properties of these emulsion-based paints, strongly connected to their colloidal organization, is essential to precise and understand artistic practices (2). We thus characterized the stability, drying properties and rheology of such binders and paints (respectively without and with dispersed pigment), sometimes also prepared with addition of lead carboxylates, common at that time.

Stable direct emulsions are generally obtained. The addition of lead carboxylates also allows the formation of stable inverse emulsions, as assessed by confocal microscopy (3). The drying mechanism of these mixed systems, explored using NMR relaxometry combined with FTIR spectroscopy, displays features of the drying of both *tempera* and oil paint. Study of their rheological properties however suggests that *tempera grassa* cannot be considered as an intermediate system between these two more conventional techniques: paints based on emulsions display distinctive flow properties (see Figure) due to their peculiar colloidal structure.

Keywords: Paint, Emulsion, Rheology, Drying

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[*] Speaker

[†] Corresponding author: come.thillaye_du_boullay@sorbonne-universite.fr

Investigating the electro-mechano-chemical coupling phenomena of an electrolyte in all solid-state battery

Kethsovann Var * [1], Christel Laberty [1], Maiza Sofiane [2], David Sicsic [3], Damien Bregiroux [1], Etienne Barthel [4]

[1] Reactive Materials for Electrochemical Systems (LCMCP-RMES) – Sorbonne Universités, UPMC, CNRS – France
[2] RENAULT – Renault - DEA-IR âĂŞ Research division âĂŞ Battery Innovation – France
[3] Technocentre Renault [Guyancourt] – Renault – Technocentre Guyancourt - 1, avenue du Golf - 78288 Guyancourt - France, France
[4] Ecole Superieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI Paris) – Université Paris sciences et lettres – 10 rue Vauquelin, 75231 Paris cedex 05, France

All solid state battery is a promising technology. However, several challenges persist, including cycling pressure, dendrite growth, and volumetric electrode variations that can lead to detachment and cracks in the electrodes, ultimately causing premature battery degradation.
This study primarily focuses on understanding the intricate relationships between electrochemical and mechanical properties within solid-state batteries. The chosen material is the argyrodite (Li6PS5Cl), which exhibits high ionic conductivity (10-3 cm-1), comparable to that of liquid electrolytes. This material can be easily compacted through cold pressing due to its favorable mechanical properties. According to literature results, the material has a relatively low Young's modulus (E) 25-40 GPa (1,2), classifying it as a soft material, in contrast to oxide families.

On the other hand we shown that the material has small elastic range, corresponding to its reversible deformation. It becomes evident that expanding the material's elastic range is imperative to accommodate electrode volumetric variations. We studied mechanical properties of argyrodite by a) modifying the particle size to manipulate macrostructural defects, and b) modifying the material's stoichiometry Li6+xPS5-x-yOyZ by introducing elements like (F, Cl, Br, I). This modification is intended to affect the strength of chemical bonds, consequently influencing the Young's modulus.

Simultaneously, on a macroscopic scale, a testing cell is developed to monitor pressure variations during cycling. The Li4Ti5O12 / Li6PS5Cl | Li6PS5Cl | Li6PS5Cl / NMC811 (single or polycrystalline) system is the primary focus. The nearly negligible volumetric variation of LTO allows for the examination of pressure changes specifically at the positive electrode. Using this system, we were able to monitor the impact of electrolyte particle size on the pressure variation. The ultimate goal is to enhance our understanding of the intricate mechanisms involved in the electro-mechano-chemical coupling and the degradation processes within solid-state batteries.

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*Speaker

Keywords: all solid state battery, nanoindentation, electo, mechano, chemical

Microscopic dynamic of Soft Particles Glasses

Chiara Marraffa * [1], Stefano Aime [1], Michel Cloitre [1]

[1] Molecular, Macromolecular Chemistry, and Materials – ESPCI Paris, PSL Research University – France

Soft particles glasses are amorphous materials composed of deformable particles jammed at volume fractions beyond close packing in a configuration where each particle is trapped in a cage formed by its neighbors with which it interacts through elastic forces.. They include many systems of industrial interest such as concentrated emulsions, microgel pastes or micelles. Despite a large diversity of composition, they share the same remarkable behavior: a transition from solid to liquid like behavior when a stress larger then yield stress is applied.
The objective of my thesis is to understand and predict the yielding properties of concentrated microgel suspensions in terms of the microstructure and particle scale dynamics. Under deformation, the particle displacements are intrinsically heterogeneous in space and time leading to strong non-affine rearrangements that are directly linked to the macroscopic yielding. However, measuring non-affine deformations in glassy materials is a very challenging task.
In this perspective, we build a novel platform consists of a custom-made parallel-plate rheometer coupled to a dynamic light scattering setup for the simultaneous measurement of the rheological properties and the microscopic dynamic. Using different mechanical history, we determine the non-affine rearrangement events under shear and we relate their dynamics to the macroscopic strain deformation. These results open promising perspectives for the investigation of the microscopic heterogeneities which play an important role in the origin of yielding, aging, and the slow relaxation of residual stresses in disordered materials.

Keywords: Soft Glasses, yielding, rheology, dynamic light scattering, non, affine dynamic

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*Speaker

03_Arranz_Maria_abstract_Rare earth-diamond hybrid structures for optical quantum technologies

Maria Alejandra Arranz *† 1

1 Institut de Recherche de Chimie Paris – Ecole Nationale Supérieure de Chimie de Paris - Chimie ParisTech-PSL, Institut de Chimie du CNRS, Centre National de la Recherche Scientifique, Ministère de la culture, Centre National de la Recherche Scientifique : UMR8247 – France

The project herein presented targets hybridization of two optically active centers of major interest for quantum technologies: Rare - earth (RE) ions in oxide thin films (1) and Nitrogen – Vacancy (NV -) color centers in diamond (2). The leading purpose will be the demonstration of NV - centers interfacing with infrared (IR) light, an unprecedent capacity whose applications span sensing, quantum processing and quantum communications.. Such hybrid structure consists of an Er3+ doped Y2O3 thin film deposited by Chemical Vapor Deposition (CVD) on a diamond substrate endowed with shallow NV-. In this work, the crystallinity of the thin film, the optical properties of the embedded Er3+ ions, and the film's impact on NV- spin and optical properties are assessed. The photoluminescence spectrum of the 4I13/2-4I15/2 Er3+ transition measured at 10 K is reported in Fig. (a) providing confirmation of the trivalent configuration of Er3+ ions in the cubic phase of Y2O3. Decay dynamics of the two Er occupational sites are shown on the inset. Values are comparable to bulk crystal references (3) which illustrates the absence of any major non-radiative or quenching effects. Figure (c) reports characterization of the optical and spin properties of the NV- before and after the thin film deposition. On the top a wide optically detected magnetic resonance (ODMR) spectrum can be observed. The 8 peaks correspond to the degeneracy lift due to 4 distinct projections of the applied magnetic field on the NV axis for two different spin projections (ms=±1). A constant linewidth, before and after deposition is observed, depicting the non altered properties of the NV- . In conclusion, the ensemble of results, act as a first proof of the possibility of integrating the rare-earth ions with NV- centers at the nanoscale level for developing hybrid solid state quantum systems

Keywords: Rare Earth ions, NV centers, diamond, quantum technologies

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[*] Speaker

[†] Corresponding author: ma.arranz-martinez@chimieparistech.psl.eu

New Oxygen Valence State in the Deep Mantle of Earth: Experimental Approach

Anne-Elisabeth Marceline * [1], Gerald Lelong† [2], Eglantine Boulard [1]

[1] Minéralogie, Pétrologie et physique planétaire [IMPMC]
(IMPMC$_{M}P3) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$
[2] Propriétés des amorphes, liquides et minéraux [IMPMC]
(IMPMC$_{P}ALM) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$

All existing geochemical models presume that oxygen (O) maintains a fixed -2 valence state in all mantle minerals (30-2900 km depth), while the redox state is traditionally allocated to the 3d transition element iron (Fe). Recent breakthroughs, however, challenge this general conception. New high-pressure phases, FeO2 and FeO2Hx (x between 0-1), have been reported under lower mantle pressure-temperature conditions, and exhibit structural similarities to pyrite (FeS2) where O substitutes sulfur atoms (S-1). Therefore, it has been proposed that these phases contain covalent O-O bonds, forming peroxide groups (O22-) with an O valence state of -1. This suggests the possibility of varying oxygen valence states, with profound implications for the modeling of Earth's deep-water cycle and interactions between the Earth's interior and atmosphere.
Nevertheless, this question is still debated, with two proposed structures: pyrite-type FeO2Hx, characterized by peroxide structures with covalent oxygen bonds and Fe2+ ions, and HP-PdF2-type FeO2Hx, featuring superoxide structures with Fe3+ ions and O-1.5. Both structures share the same space group (Pa3 éĚ), with differences in the oxygen atomic position. X-Ray Diffraction (XRD) alone has not been sufficient to conclusively determine the crystallographic structure.

This study aims to directly assess the presence/absence of covalent O-O bonds employing InfraRed and Raman spectroscopy on FeO2Hx samples synthesized from different precursors and characterized by XRD. In addition, Raman spectra were collected on various peroxide standards under compression to the same pressure range. Our results show that FeO2Hx Raman spectra reveal two modes at 90 GPa, within the expected O-O wavenumber range.
Secondly, high-pressure XRD investigations on different chemical/mineral systems were undertaken to study the interaction between FeO2Hx with major mantle minerals to bring light on the stability field of FeO2Hx in the lower mantle of the Earth and explore the possibility of solid solutions with major cations from the Earth's mantle.

Keywords: Deep Earth, Geochemistry, Crystallochemistry, Planetology, Structure & history of the Earth, Deep water cycle, XRD, Spectroscopy

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*Speaker

†Corresponding author: gerald.lelong@upmc.fr

A tunable MOF platform for chiral chromatographic separations

Soraya Bouras * [1,2], Cédric Boissière [3], JérÃťme Vial [2], Didier Thiebaut [2],
Christian Serre [1], Antoine Tissot† [1]

[1] Institut des Matériaux Poreux de Paris (IMAP) – Ecole Normale Supérieure de Paris - ENS Paris, ESPCI Paris, PSL Research University, CNRS : UMR8004 – 75005 Paris, France
[2] LSABM Chimie-Biologie-Innovation (UMR 8231) (CBI) – Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Centre National de la Recherche Scientifique – 75005 Paris, France
[3] Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – 75005 Paris, France

Current stationary phases used in chiral High-Performance Liquid Chromatography (HPLC) or Supercritical Fluid Chromatography (SFC) mainly rely on the use of functionalized cellulose or amylose. They allow efficient separation of many chiral mixtures but their cost remains excessively high regardless of the column.
MOFs are a class of porous hybrid crystalline solids promising for many applications related to gas separation/storage, catalysis, environment and health among others, thanks to their high porosity combined with a wide range of possible functionalization.1

The use of MOFs as stationary phases has been investigated within the past decade but the same issues remain: low column efficiency and excessive column backpressure have been reported as a result of the irregular shape, sub-micrometer and wide size distribution of the MOFs particles.2,3

Therefore, this project aims to design for the first time a tunable platform of cheap and efficient pure MOF chiral stationary phases for chromatography through the preparation of mesoporous MOFs, bearing specific affordable chiral groups, shaped through spray-drying as mechanically stable micrometric particles.

The MOF selected for this study, MIP-206, is a zirconium oxoclusters based mesoporous solid built with substituted feedstock derived isophthalic acids (IPA) whose large 1D pores (2.6 nm) offer an ideal platform for chromatographic separation. Along with their high chemical stability, MIP-206s can be modified with functional groups either through ligand modification or by grafting onto Zr(IV) sites in the pores4.
MIP-206 has first been functionalized through post-synthesis modification (PSM) with a chiral group, camphorsulfonic acid (CSA). MIP-206/CSA was then shaped by spray-drying into âĂŸdoughnuts' like particles and packed into a HPLC column under 200 bars. As first result, the obtained column demonstrated a separation of carvone enantiomers with a promising selectivity of more than 1.2.

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[*] Speaker

[†] Corresponding author: antoine.tissot@ens.psl.eu

Keywords: Metal Organic Frameworks, Chiral Chromatography, Spray drying, Separation

Metal-Organic Frameworks for Hydrogen Production through Light-driven Overall Water Splitting: XAS for Deeper Insights

Edouard VÃűgtli *† [1], Anthony Beauvois [2], Georges Mouchaham [3], Laurent Barthe [2], Antoine Tissot [3], Sergio NavalÃşn [4], Hermenegildo GarcÃŋa [4], Valérie Briois [2], Christian Serre [3]

[1] Ecole Superieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI Paris) – Université Paris sciences et lettres – 10 rue Vauquelin, 75231 Paris cedex 05, France
[2] Synchrotron SOLEIL (SSOLEIL) – Centre National de la Recherche Scientifique – L'Orme des Merisiers Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX, France
[3] Institut des Matériaux Poreux de Paris (IMAP) – Département de Chimie - ENS Paris, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Institut de Chimie du CNRS, Centre National de la Recherche Scientifique – ENS, 24 rue Lhomond et ESPCI, 10 rue Vauquelin, 75005 Paris, France
[4] Universitat Politècnica de València = Universitad Politecnica de Valencia = Polytechnic University of Valencia (UPV) – Camino de Vera, s/n 46022 Valencia, Spain

H2 is among the most attractive chemical energy carriers to replace fossil fuels. It possesses the highest energy density per unit mass, almost three times higher than gasoline, and has water as unique combustion product.(1) However, non-sustainable fossil fuel dependent processes still account for most of the worldwide hydrogen production.(2) In the search of alternatives, solar energy assisted water splitting, a green technology, is of particular interest. Metal-Organic Frameworks (MOFs) -porous crystalline organic-inorganic solids- are drawing increasing interest in catalysis, owing to their tunable structure and physicochemical properties.(3) Numerous reports deal with MOFs for photocatalytic water splitting but suffer from either a lack of solar-to-hydrogen (STH) conversion efficiency and/or stability under operation.(4) Understanding the underlying mechanism is key to steer the conception of new generations of catalysts of improved performance. In this regard, X-ray Absorption Spectroscopy (XAS) is a powerful technique to investigate the atomic electronic and local structures. When it is used under *operando* conditions, it allows to monitor the evolution of the active site(s) enabling deep insights all over the targeted reaction. Here, we report an efficient Cu/Zr bimetallic MOF-based photocatalyst for OWS, the conception of a new photochemical cell, and the monitoring of the Cu and Zr electronic states and coordination environment under *operando* conditions.

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(2) *Energy Fuels,* 2021, 35, 20, 16403–16415

(3) *Chem. Rev.* 2010, 110, 8, 4606–4655
(4) *Chem. Rev.* 2023, 123, 1, 445-490

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[*] Speaker
[†] Corresponding author: edouard.vogtli@espci.fr

Keywords: MOF, Metal, Organic Framework, Hydrogen, OWS, Overall Water Splitting, Water Splitting, XAS, X, ray Absorption Spectroscopy, Catalysis, Spectroscopy

Towards Neuromorphic Computing: VO2 Transition Dynamics

Melissa Alzate Banguero * [1], Lionel Aigouy [2], Alexandre Zimmers [2], Erica Carlson [3]

[1] LPEM, ESPCI – ESPCI Paris, PSL Research University – France
[2] LPEM, ESPCI – CNRS, UPMC, ESPCI – France
[3] Purdue University – United States

The current state of AI algorithms involves their implementation in silicon-based computer architectures. However, to fully realize the potential of AI, it is crucial that these underlying architectures more closely emulate the synapses and neurons found in the human brain. While numerous materials are being considered for mimicking synapses, only a few quantum materials are suitable for replicating the behavior of neurons. These materials exhibit intricate, multiscale structures that are highly responsive to stimuli, resembling the electrical spikes observed in brain activity.

Transition metal oxides have emerged as promising candidates in this pursuit. Over recent years, phase separation phenomena in these oxides have been revealed spanning from the nanometer to micron scales. This breakthrough has enabled the extraction and analysis of critical parameters such as cluster size and critical exponents at various temperatures during the transition. However, fine-scale changes in cluster dynamics during a slow temperature sweep have remained a challenge to track.

To address this, we have developed a variable temperature autofocus microscope capable of operating within the range of 77K to 600K, utilizing visible light. This allows for the acquisition of up to 1000 images while crossing the critical temperature (Tc). We have chosen the quantum material VO2 since its metal-to-insulator transition occurs near room temperature, and it exhibits non-volatile memory and neuron-like behavior.

In this work, we introduce the experimental setup and image analysis developed to achieve this study. We also present key results obtained on Vanadium Dioxide, VO2: critical temperature maps (Tc maps), hysteresis maps, memory maps, avalanches, and pattern recognition of clusters using machine learning.

Keywords: neuromorphic computing, insulating to metal transition, quantum material, memory, optical characterization

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*Speaker

Optimizing synthesis conditions of magnesium silicates as selective catalysts for the GVL ring-opening reaction

Albert Issa * [1,2], Guillaume Laugel [1], Thomas Onfroy [1], Jean-FranÃğois Hochepied [2], Hélène Lauron-Pernot [1]

[1] Laboratoire de Réactivité de Surface (LRS) – Laboratoire de Réactivité de Surface (LRS-UMR 7197, UPMC-CNRS), Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, France – 4 Place Jussieu, 75005, France

[2] Ecole Nationale Supérieure de Techniques Avancées (ENSTA Paris) – ENSTA-Paris, UCP, Palaiseau 91120, France – 828, boulevard des Maréchaux 91762 Palaiseau Cedex, France

Transesterification reactions are used in various applications in the field of valorizing bio-based molecules. For instance, the opening of γ-valerolactone (GVL) with methanol leads to the formation of methyl pentenoates, which are used as intermediates in nylon synthesis (figure 1). Preliminary studies have highlighted the advantages of using magnesium silicates (MS), which have acid-base surface properties, as catalysts in model transesterification reactions (1). However, it has also been shown that the synthesis route plays a crucial role in the catalytic performance (1).

The coprecipitation of MS was carried out using two synthesis methods: one involved a micro-mixer allowing rapid mixing in about 10 milliseconds (2), and the other used a double-jet batch system, which provided longer mixing times but allowed precise control of pH and temperature. A parametric study was conducted to determine the influence of several synthesis parameters, including pH, temperature, and the synthesis method (micro-mixer or double jet), on the final properties of the MS.

An experimental dataset, obtained through N2 physisorption, scanning electron microscopy (SEM), XRD, indicates a strong influence of the synthesis method on the specific surface area obtained. The silicates prepared in the micro-mixer with a final Mg/Si ratio $>$ 0.7 have a monolithic structure (Figure 2(a)) and do not possess any measurable surface. When the double-jet reactor was used for synthesis, this lack of measurable specific surface area could be overcome: samples prepared under the same conditions thus have high specific surface areas ($>$ 150 m2/g). The final ratio of magnesium (Mg) to silicon (Si) in the solid materials, influenced by the synthesis process, pH, and temperature, significantly impacts the acid-base properties of these solids. As the Mg/Si ratio increases, the selectivity for MP4 also increases, while the trend is the opposite for other products.

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[*] Speaker

Mesoionic carbenes, innovative ligands for the stabilization of plasmonic nanoparticles

Salem Saleh Salem Ba Sowid * [1,2], Alexandre Porcheron [3], Omar Sadek [4], Nathalie Bridonneau [5], Laura Hippolyte [3], Dimitri Mercier [6], Philippe Marcus [6], Lukmonjon Mutalliev [7], Clément Chauvier [7], Chaneac Corinne [5], Louis Fensterbank† [7], Francois Ribot‡ [5]

[1] BA SOWID Salem – Sorbonne Universités, UPMC, CNRS, LCMCP, Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France – France
[2] LCMCP, IPCM – SORBOONE UNIVERSITY-UPMC – France
[3] LCMCP, IPCM – Sorbonne Universités, UPMC, CNRS – France
[4] IPCM – SORBOONE UNIVERSITY-UPMC – France
[5] LCMCP – Sorbonne Universités, UPMC, CNRS – France
[6] IRCP – Institut de Recherche de Chimie Paris - IRCP – France
[7] IPCM – Sorbonne Universités, UPMC, CNRS – France

Stabilization of plasmonic nanoparticles in colloidal suspension to ensure their functionality in several applications such as nanocatalysis, nanomedicine, and electronics is a crucial challenge. Thiol-based ligands have been conventionally employed to stabilize gold nanoparticles (AuNPs). However more recently, N-heterocyclic carbenes (NHCs) have gained interest as strong-binding surface ligands that can outperform thiols. While classical NHCs, based on (benz)imidazole, can be modularly synthesized, time-consuming multi-step synthesis is needed to achieve unsymmetrical or functionalized NHCs. Mesoionic carbenes (MICs) on the other hand are robust subclass of NHCs. Unlike classical NHCs, MICs can be easily synthesized via simple copper-catalyzed alkyne-azide click (CuAAC) reaction followed by alkylation step, which allows to introduce up to three different functions on the MIC core. Moreover, MICs are stronger σ-donors than the classical NHCs, which offers higher stability to the nanoparticles. Herein, a simpler alternative, a one-pot straightforward synthesis of MIC-stabilized AuNPs directly from 1,2,3-triazolium salts and tetrachloroauric acid is reported. In this study, a library of MIC precursors was synthesized from which a series of stable MIC-AuNPs could be isolated. The effect of the nature of the MIC precursor as well as the triazolium/gold ratio were shown to have a direct effect on the size of AuNPs, as demonstrated by TEM studies. X-ray photoelectron spectroscopy (XPS) was used to characterize the nanoparticles' nature and confirm the presence of MICs as capping ligands on the AuNP surface. These MIC-AuNPs were demonstrated to be stable to storage in solution for months, to low/high temperatures, and to the presence of high concentrations of exogenous thiols. In addition, the catalytic activity of these nanoparticles for the reduction of nitrophenol was explored. This work showcases a modular and practical one-pot synthesis towards robust MIC@AuNPs which does not require pre-isolation of MIC-gold complex or triazolium-gold salt.

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*Speaker

†Corresponding author: louis.fensterbank@sorbonne-universite.fr

‡Corresponding author: francois.ribot@sorbonne-universite.fr

Langmuir films of Perfluoroalkylalkanes: what drives apolar molecules to form monodisperse and organised surface aggregates

Pedro Silva *† [1,2], Eduardo Filipe [1], Pedro Morgado [1], Marie-Claude Fauré [2,3], Michel Goldmann [2,3,4]

[1] Centro de Quimica Estrutural (CQE) – Complexo I, Instituto Superior Técnico, Technical University of Lisbon, Av. Rovisco Pais, 1049-001 Lisbon, Portugal, Portugal
[2] Institut des Nanosciences de Paris (INSP) – Sorbonne UniversitéĄ, Centre National de la Recherche Scientifique – Sorbonne-Université, Case 840 4 place Jussieu 75252 Paris Cedex 05, France
[3] UFR Sciences Fondamentales et Biomédicales [Sciences] - Université Paris Cité – Université Paris Cité – Campus Saint-Germain-des-Prés - 45 rue des Saints Pères - 75006 Paris, France
[4] Synchrotron SOLEIL (SSOLEIL) – Centre National de la Recherche Scientifique – L'Orme des Merisiers Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX, France

Perfluoroalkylalkanes (CnF2n+1CmH2m+1 or FnHm) are diblock molecules formed by a hydrogenated (CH) chain linked to a perfluorinated (CF) segment. Both are hydrophobic and mutually phobic. Despite lacking a polar group, it's been known for over 30 years that these primitive surfactants can form Langmuir films on water or hydrophilic substrates. The films comprise well-defined, monodisperse hemimicelles.
The aim of this work is to quantitatively characterise the hemimicelles' structure and organisation at the air–water interface, as well as to determine the fundamental principles driving this spontaneous and remarkable self-assembly phenomenon. This is pursued in a two-pronged approach, combining computational (Molecular Dynamics (MD) simulations) and experimental (Surface Pressure-Molecular Area (pi–A) isotherms, Grazing Incidence X-Ray Diffraction (GIXD) and Scattering (GISAXS), Atomic Force Microscopy (AFM)) methods.

MD simulations have been used to model these systems, elucidating the geometrical and energetic factors determining the hemimicelles': inner structure; size, depending on the length of the CH/CF chains; origin of their central pit as a consequence of the ordering of the CH2-CF2 dipoles and concomitant deformation of the water surface.

Experimental studies have been focused on: a) changing the liquid water subphase for short-chain alcohols; b) characterising water-supported mixed binary films of FnHm. Both cases serve as model systems to probe the effect of varying dipole-dipole/dispersive interactions on the structure, mixing and ordering of the films. It has been established that: ordered hemimicelles can form at the surface of short-chain alcohols; mixing occurs within the binary films, comprising hemimicelles that form a hexagonal lattice with a size intermediate of that of the pure ones.
The obtained results are promising and, taken together, they have been rationalised as the consequence of the subtle balance of the intermolecular interactions happening at the interface.

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[*] Speaker

[†] Corresponding author: pedro.ribeiro.silva@tecnico.ulisboa.pt

Ultimately, these may serve as tunable parameters to control the self-assembly process for practical applications.

Keywords: Perfluoroalkylalkanes, Langmuir Films, Molecular Dynamics Simulations, AFM, GISAXS, GIXD

Prebiotic synthesis pathays by ab initio, machine learning, and stochastic molecular dynamics.

Léon Huet * [1,2], Marco Saitta [2], Fabio Pietrucci [2], Rodolphe Vuilleumier [3]

[1] Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC) – Institut de minéralogie, de physique des matériaux et de cosmochimie, CNRS : UMR7590, Université Paris VI - Pierre et Marie Curie, Muséum National d'Histoire Naturelle (MNHN) – 4, place Jussieu - Tour 23 - Barre 22-23, 4e étage - 75252 Paris Cedex 5, France
[2] Physique des systèmes simples en conditions extrêmes [IMPMC] (IMPMC$_PHYSIX) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie - -4, placeJussieu - BC115 - 75252ParisCedex5, France$
[3] Département de Chimie - ENS Paris – Ecole normale supérieure - Paris – 24 rue Lhomond75132 Paris Cedex 05, France

In contemporary prebiotic chemistry, advanced modeling protocols are indispensable. They underpin experimental progress and explore novel compounds and mechanisms.
To overcome human interpretation, these tools must be agnostic and transferable. Two such tools, enhanced sampling methods and machine learning interatomic potentials, have already been applied to investigate the glycine synthesis mechanism. Their usage led us to the discovery of an alternative pathways toward glycine, distinct from the commonly discussed "Strecker mechanism" of the literature. We have conducted a thorough characterization of this new pathway for the purpose of comparison.

However, a significant challenge remains in accurately estimating reaction kinetics to determine which pathway is the primary one. This underscores the need for further developments. Our proposed solution is to use the data from our prior studies and incorporate it into a dynamic model known as the 'Generalized Langevin Equation'. This model wil emulate the dynamic behavior of the entire system in order to provide a more accurate measurement of the reaction speed.
Such approach promise to improve kinetics estimation in a field where reaction time is a critical factor.

Keywords: prebiotic chemistry, molecular dynamics, stochastic sampling

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*Speaker

Degradation of organic pollutants by a new eco-compatible process: kinetic approaches at the surface-water interface

Ana Carolina Schuh Frantz * [1,2]

[1] Laboratoire de Réactivité de Surface (LRS) – Institut de Chimie du CNRS, Sorbonne UniversitéĄ,
Centre National de la Recherche Scientifique – Tour 54- 2ème etg 4 Place Jussieu - Case 178 75252
PARIS CEDEX 05, France
[2] Minéralogie Environnementale [IMPMC]
(IMPMC$_M$$INENV) - -Institutdeminralogie, dephysiquedesmatriauxetdecosmochimie -$
$-4, placeJussieu - BC115 - 75252ParisCedex5, France$

The presence of organic pollutants in the environment evoke toxicological concerns to public health and biodiversity due to their inherent carcinogenic properties. A major issue is related to the difficulty to degrade these chemicals, such as insecticides, herbicides, plasticizers, antibiotics, and chlorinated solvents, that therefore end-up into groundwater and may accumulate in soils. To overcome this issue, efficient and scalable remediation methods are needed to control long-term impacts to ecosystems. Advanced oxidation processes (AOPs) offer solutions for wastewater management, by hydroxyl radicals production, under multiple approaches, such as photocatalysis, electrochemical technologies, ozone-based processes and many others. In this work, we are particularly interested in Fenton-based reactions as AOP to reach organics degradation, where the materials used are synthetic nano-magnetite, as catalyst, and nalidixic acid, a pharmaceutical pollutant. The key point is to explore iron oxide ability to produce hydroxyls via the Fe(II)/Fe(III) oxidation cycle to degrade poorly biodegradable contaminants. Nevertheless, applicability to natural environments is a priority, which is why all experiments are carried out in neutral pH and the catalytic process is triggered by less aggressive oxidation agents, such as air-borne or pure oxygen. The main challenge in this project lies in both the understanding of the reaction mechanism and the complexity of the in-situ characterization. A new set-up was developed by our team in order to investigate heterogeneous catalysis triggered by oxygen, which requires controlled working space, under constant water-flux. As the main characterization method, we are using Rapid Scan Infrared Spectroscopy in Attenuated Total Reflectance mode (i.e., ATR-FTIR) since it allows us to investigate substrate-water interface over time. Experiments are carried step by step: (i) water flow stabilization, (ii) nalidixic acid adsorption onto magnetite, and (iii) sorbed molecules' reduction due to substrate oxidation. So far, the experimental parameters have been established, leading to reproducible stabilization and adsorption steps, but there are yet challenges to overcome regarding the catalytic degradation triggered by O2 and its spectral interpretation.

Keywords: ATR, FTIR, spectroscopy, characterisation, heterogeneous catalysis, Fenton, like

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[*] Speaker

Insertion of synthetic nanopores into polymeric membranes

Yang Yu * [1], Haiqin Du [2], Wencui Zhang [3], Fernando Giacomelli [4], Cécile Huin [3,5], Philippe Guégan† [3]

[1] IPCM – Sorbonne Universités, UPMC Univ Paris 06 CNRS Institut Parisien de Chimie Moléculaire, UMR 8232 Chimie des Polymères – France
[2] State Key Laboratory of Molecular Engineering of Polymers, Fudan University, Shanghai, China. – China
[3] IPCM – Sorbonne Universités, UPMC Univ Paris 06 CNRS Institut Parisien de Chimie Moléculaire, UMR 8232 Chimie des Polymères – France
[4] Centro de CiÃłncias Naturais e Humanas, Universidade Federal do ABC, Santo André – Brazil
[5] University of Evry – University of Evry, University of Evry – France

The generation of biomimetic nanopores and nanochannels inspired by ion channels is an exciting area of scientific research, as such biomimetic materials serve as fundamental platforms that may inspire experimental and theoretical efforts to model the processes of ion transport in vivo and Enhance the function of biological ion channels and promote the development of bionic smart nanopore/nanochannel devices in the fields of biosensors, nanofluidic devices and molecular filtration.

We hope to develop a robust system that mimics natural cells by inserting synthetic nanopores into polymer membranes. Our interest in polymer membranes is based on their longer stability compared to lipid bilayers and the possibility to tune the membrane thickness by changing the molar mass of the polymer blocks.

Our approach is to design a library of (co)polymers capable of forming planar polymer membranes and/or polymersomes, and to design macrocycle-based synthetic nanopores that enable predefined permeability structures.

The synthetic part is achieved through a combination of organic chemistry and polymerization reactions. Characterization of objects by NMR, GPC and MS. The self-assembly of objects in solution was evaluated by dynamic light scattering and finally by SAXS and cryo-TEM. The ability to insert synthetic nanopores into polymeric membranes was evaluated by electrical detection using black lipid membrane technology.

We have demonstrated that polymersomes can be obtained from cyclodextrin-based star polymers with a chemical structure close to that of chemical nanopores. Permeation studies were performed and it was observed that translocation is dependent on the chemical nature of

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*Speaker

†Corresponding author: philippe.guegan@sorbonne-universite.fr

the analyte. The pioneering results are now expected to be expanded upon and their applications in chemistry and the natural sciences envisaged.

Optimization of the fabrication processes of Nd-Fe-B permanent magnets by the CALPHAD method

Eloi De Villoutreys * [1], Andrea Quaini [1], Jean-Louis Flèche [1], Cyril Rado [2], Stéphane Gossé [1]

[1] Service de recherche en Corrosion et Comportement des Matériaux (S2CM) – Département de Recherche sur les Matériaux et la Physico-chimie pour les énergies bas carbone – France
[2] Département des Technologies des NanoMatériaux (DTNM) – Laboratoire d'Innovation pour les Technologies des Energies Nouvelles et les nanomatériaux – France

The strong worldwide demand for Nd-Fe-B permanent magnets and the criticality of Neodymium (Nd) are driving manufacturers to develop new magnets in which Nd is partially replaced by other less critical Rare Earths (RE) such as Cerium (Ce) or Lanthanum (La). The development of these new substituted magnets requires fine control of the microstructure, especially the distribution of phases at grain boundaries. This complexity calls for the development of a numerical approach to the thermodynamics of these systems. The primary aim of this project is to reach an optimum between a Nd-reduced composition in favor of non-critical REs and a microstructure that guarantees high magnetic performance; essentially, an optimum between a composition and a manufacturing process.

This thesis focuses on the evolution of the Nd2Fe14B main phase and grain boundary phases by the addition of Ce and other REs into the system. Some phases, such as the Nd-rich phases, are necessary to maintain coercitivity in the magnet, while others, such as FeB, have adverse effects on magnet properties. Non-intuitively, the presence of the paramagnetic CeFe2 phase may help maintain magnet coercivity by enhancing the wettability of the 2:14:1 phase.

An experimental study and modeling were carried out on the (Ce,Nd)-Fe-B system using the CALPHAD method. This method consists in modeling all Gibbs energy functions of the system phases in order to reproduce the experimentally observed thermodynamic equilibria and properties. Annealed samples were subjected to EDS and EPMA analysis. DTA and quasi-harmonic calculations were performed to obtain missing fundamental data. Application calculations have also been carried out with the under development thermodynamic model to propose first directions of relevant compositions to the elaboration of future substituted magnets.

Keywords: Permanent magnet, Thermodynamic, Phase equilibria, CALPHAD

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*Speaker

Ionic Exchange in a Phase-Separated Glass

Anais Verron * [1,2]

[1] Unité Mixte CNRS/Saint-Gobain - Surface du Verre et Interfaces – Ekaterina Burov, Barbara Bouteille – France
[2] PMMH, ESPCI – Damien Vandembroucq – France

Diffusion on glass material plays a key role in industrial and geological processes. Many models and mechanisms have been developed and gives us a better understanding on how diffusion works. However, few experimental studies have been reported so far on the diffusion of ions in a heterogeneous media. The present study investigates how heterogeneities in composition impact interdiffusion.

The works consist in performing silver and copper-based ion exchange in a phase separated borosilicate glass. Some borosilicate glass separates into two glassy phases: an alkali-rich phase and a silica-rich phase. The aim of the thesis is understanding how the differences in composition, chemical and physical properties between the two phases impact the diffusion of metallic ions.

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*Speaker

Bringing Infrared Spectroscopy into Batteries with Optic Fibers

Cédric Leau * [1,2,3]

[1] Chimie du Solide et de l'Energie (CSE) – Chimie du Solide et de l'Energie - Collège de France – Collège de France, Paris, France
[2] Réseau sur le Stockage Electrochimique de l'Energie (RS2E) – Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, France – France
[3] Sorbonne UniversitÚniversité , CNRS – France

Electric mobility is one of the technological option available to mitigate climate change, but limited understanding of battery degradation poses a significant challenge in achieving sustainable and reliable energy storage. Thus, recent research efforts focus on providing an experimental framework to monitor batteries over their lifespan, to extend their longevity (1). Huang *et al.* demonstrated how optic fiber sensors implemented in battery cells could provide local measurement of temperature, strain and refractive index variations (2, 3), providing valuable insights into the battery's behavior. To gain richer molecular-level knowledge of the battery chemistry, we developed an approach based on Infrared Fiber Evanescent Wave Spectroscopy (IR-FEWS), working *operando*.

Chalcogenide glass optic fibers displaying mid-IR transparency were implemented in various battery systems. Our experimental results show the feasibility of monitoring the stability of salts and solvents in various electrolytes over cycling. When directly embedding the fiber within the electrode, we observed the lithiation of IR-active material (3). We also evidence several species constitutive of the Solid Electrolyte Interface (SEI), which plays a critical role in governing battery performances. A numerical analysis based on Alternate Least Square method is conducted to distinguish contributions of the electrolyte from those of the SEI.

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[*] Speaker

Influence of interface dipole on charge build-up under high voltage

Lin Zheng * [1]

[1] Laboratoire de Physique et d'étude des Matériaux (UMR 8213) – CNRS, UPMC, ESPCI – France

Interface dipole was measured in various polyethylene samples with a high sensitive pressure-wave-propagation measurement setup under low voltage (30 V/mm at most). Larger samples were taken from the same polyethylene specimens with different coatings and subjected to high voltage (40 kV/mm) for 24 h to detect charge build-up at 22 ○C. In this paper, charge evolution is discussed in relation with the measured interface dipoles. Correlations between interface dipole and charge build-up are clearly observed.

Keywords: interface dipoles, space charge, pressure, wave, propagation (PWP) method, polyethylene

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[*] Speaker