

POROUS SOLIDS: UNITY IN DIVERSITY

**RESPORE INTERNATIONAL
CONGRESS**



ONLINE **JUNE 16-17 2021** **PROGRAMME**

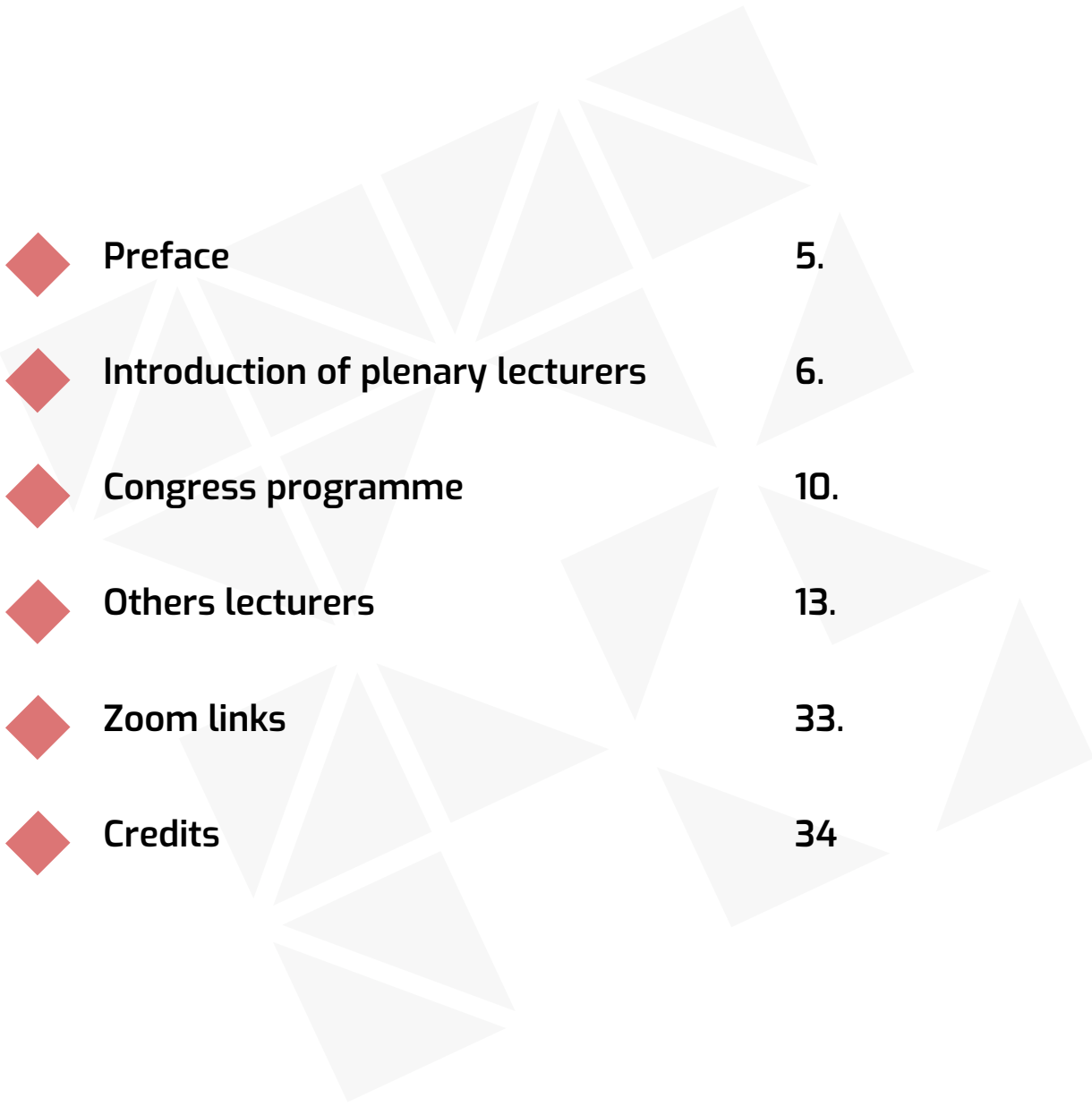
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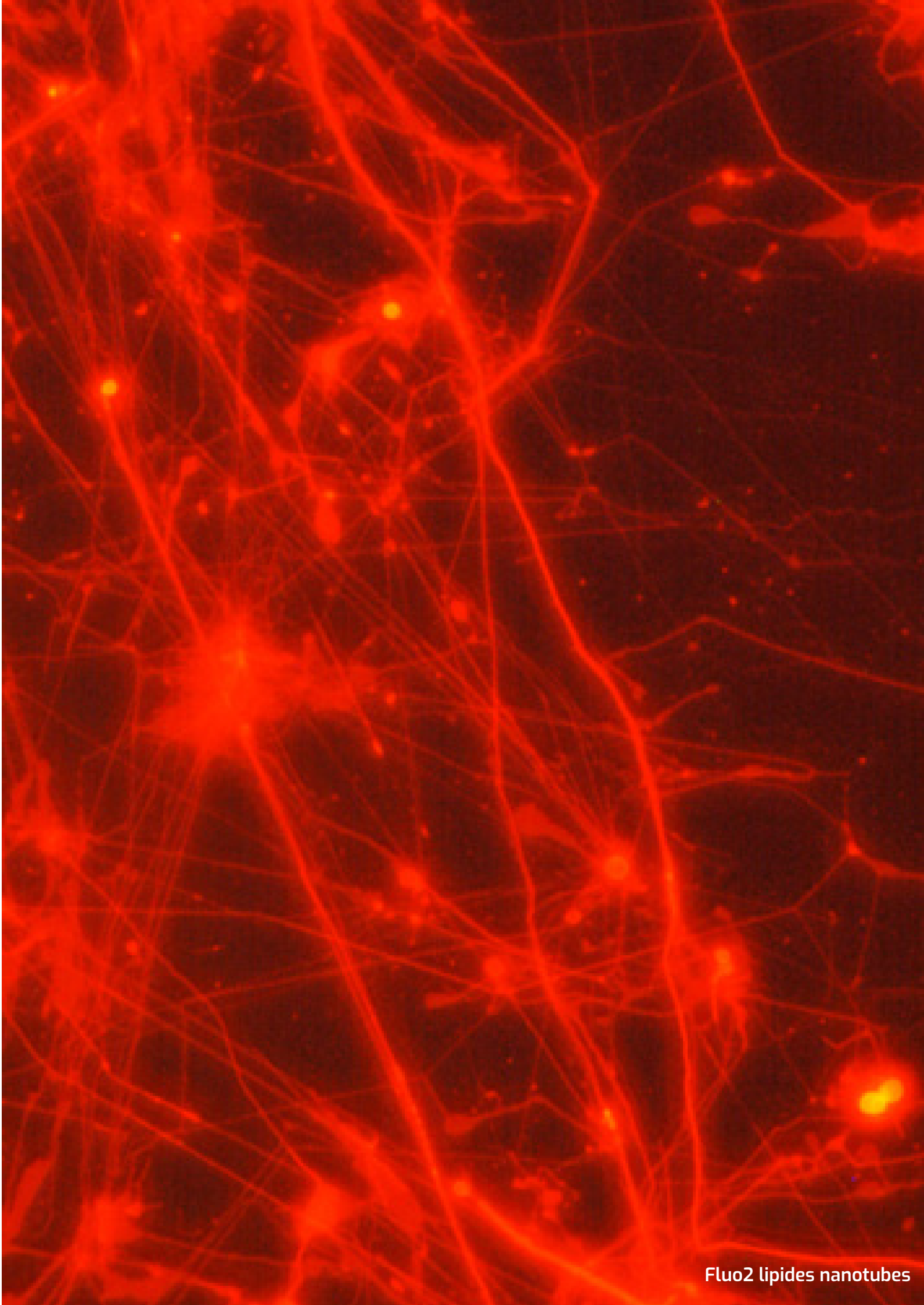
RESPORE
Réseau d'excellence en solides poreux



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Preface

Porous solids, whether molecular or extended, of biological, mineral, carbon or hybrid nature, are fascinating materials due to their great chemical and structural diversity and their potential to respond to societal challenges in health, energy or the environment. The Domain of Major Interest (DMI) of the Ile-de-France region 'Respore' aims at going beyond the simple multidisciplinary between chemists, physicists, biologists and medicine; with both breakthrough approaches at the interface of the different classes of porous solids but also by transferring concepts and or approaches from one disciplinary field to another. The "Porous solids: unity in diversity" conference on 16th and 17th June 2021 will illustrate this approach through a high-level scientific meeting between renowned international speakers and actors of the DIM Respire.

Christian Serre

Research director (ENS, ESPCI, PSL, CNRS)

Juan Pelta

Professor (Cergy, Evry)

Jean-Marie Tarascon

Professor (Collège de France)

Keynotes speakers

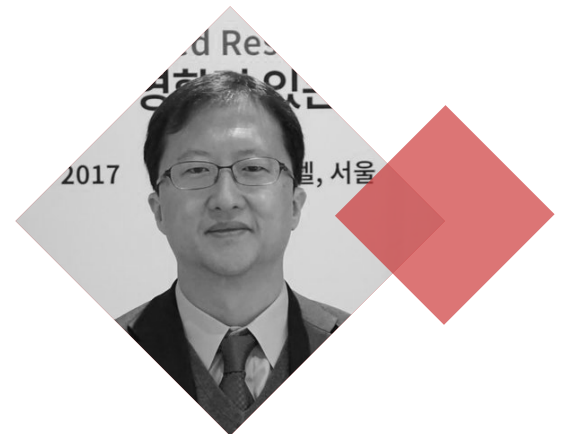


Silvia Bordiga

Department of Chemistry and NIS Centre,
University of Turin, Italy

Catalytic materials under investigation through the eye of a spectroscopist

Cu-exchanged chabazite (Cu-CHA), currently widely used in NH₃-assisted selective catalytic reduction (SCR) of NO_x, is considered a case study to show crucial points in the investigation of heterogeneous catalysts through in situ and operando spectroscopies. What are the strengths and weaknesses of some of the most used techniques and what is the role of molecular modeling in supporting the understanding of the system under consideration? How relevant is the availability of a set of samples with a well-defined structure and composition in order to identify general trends in the catalytic behavior of the catalysts? How is it possible to perform a structure-catalytic properties correlation to develop new catalysts with better performances?



Jang Wook Choi

School of Chemical and Biological Engineering,
Seoul National University, Republic of Korea

Advanced binder designs for sulfide-based all solid-state batteries

Although Lithium-ion batteries (LIBs) have successfully powered various applications, they are evolving continuously for further improved performance in many aspects. Beside LIBs, other post-LIBs have been intensively studied as complementary options, and all-solid-state-batteries (ASSBs) are receiving discernable attention due to their superiority in safety. In particular, in response to this trend related to those emerging batteries, new binder designs are demanded. In this talk, I will present some binder designs targeting sulfide-based ASSBs. I will first introduce the difficulty of finding solvent-binder pairs compatible with sulfide electrolytes and will then cover our recent process on how to avoid the given problem. The incompatible polarity among binder, sulfide solid electrolyte, and slurry solvent requires novel approaches in the electrode fabrication process. Along this direction, I will introduce binder designs based on click and deprotection chemistry. These approaches allow one to avoid the compatibility issue and achieve as high electrode adhesion as that in the LIBs, along with superior cycling performance.



Alexander V. Neimark

Department of Chemical and Biochemical Engineering, Rutgers University, New Jersey, USA

Advanced characterization of structural and adsorption properties of metal-organic frameworks

Pore structure characterization and coupling of adsorption and structural properties of MOF materials are imperative for their design, fabrication, quality control, and practical applications. The pore structure of MOF crystals represents a three-dimensional network comprised of several types of pore compartments: interconnected cages and channels distinguished by their size, shape, and chemistry. Here, we propose a novel methodology for pore structure characterization based on matching the experimental adsorption isotherms to in-silico generated fingerprint isotherms of adsorption in individual pore compartments of the ideal crystal. This approach allows to elucidate the adsorption mechanisms, determine the contributions of different pore compartments into the total adsorption, and estimate to what extent the pore structure of the sample under investigation is different from that of the ideal MOF crystal. The pore structure is characterized by the pore type distribution (PTD), which is more informative than the traditional pore size distribution that is based on oversimplistic pore models. The proposed methodology is illustrated on examples of Ar, N₂, and CO₂ adsorption on four structurally distinct MOF materials: Cu-BTC, UiO-66, PCN-224, and ZIF-412. The PTD determined from the experimental isotherm provides an estimate of the crystal fraction in the sample, accessibility and degree of hydration of different types of pore compartments. In addition, the PTD determined from the experimental adsorption isotherm is used to predict the isosteric heat of adsorption that provides important information on the energies of adsorption interactions. The results are found in excellent agreement with experimental data on adsorption isotherms, isosteric heats, and adsorbate density distributions between different pore compartments obtained by in situ XRD crystallography [2].

[1] S. Dantas et al., JACS, 141 (2019) 8397; ACS AM&I, 12 (2020)15595.

[2] H. S. Cho et al., Nat. Chem. 11 (2019) 562



Yi Tao Long

School of Chemistry and Chemical Engineering, Nanjing University, China

Nanoconfinement controlled chemistry for single -molecule sensing

Single molecule sensing using biological nanopore has greatly enhanced the precision and depth of our knowledge about living system. The million years of evolution have produced the membrane proteins which acts as a single biomolecule interface for capturing and identifying a single molecule of interests. This sensing interface in a pore nanostructure could be adapted for highly sensitive electrochemical sensing. Currently, we focus on the nanoconfined controlled electrochemical method for single molecule measurements.[1-3] We outline the design of nanoconfined-based single biomolecule interface which provides rich heterogeneities and stochastics information about each molecule. Then, we focus on the future areas beyond DNA sequencing including detecting rare species, resolving the hidden intermediates, depicting the spectra for the covalent/non-covalent interactions, tracing the dynamic pathways of single molecule proteins.[4-6] A concept "single-molecule ionic spectrum" could potentially map the non-covalent interaction at atomic level in future. Since the characteristic interaction among the amino acids in nanopore channel determines the sensing sensitivity, ideally the frequency analysis of nanopore ionic current could potentially allow discriminate each amino acid. As ideally transferring the frequency-energy spectrum from the ionic current into the voice frequency, we illustrate that a nanopore-based single-biomolecule interface likes a 'tuba'. When the single analyte flows into the 'tuba', its dynamic interaction with the pore could be modulated by the residue of the pore ('button') and the resonance space at the single-molecule interface ('tuba'). As a result, the beautiful music of a single molecule will be played with a typical rhythm and melody.

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6.M.-Y. Li, Y.-L. Ying, J. Yu, S.-C. Liu, Y.-Q. Wang, S. Li, Y.-T. Long, Revisiting the Origin of Nanopore Current Blockage for Volume Difference Sensing at the Atomic Level, JACS Au, DOI: 10.1021/jacsau.1c00109

Programme

Day 1

9h	Opening	
9h15	Keynote Jang Wook Choi	Advanced binder designs for sulfide-based all solid-state batteries
10h	Invited Robert Dominko	Bio sourced membranes as interlayers in Li batteries
10h25	Pause	
10h55	Invited Jan Carmeliet	Anomalous water transport in multiscale porous materials like textiles
11h20	Invited Chris McMin	Fluid-fluid phase separation in a soft porous medium
11h45	Flash pres. Clement Campillo	Mechanics of micropatterned cancer cells by AFM
11h55	Flash pres. Abelghani Oukhaled	On single-molecule protein sequencing through nanopores: challenges and opportunities
12h05	Flash pres. Nathalie Jarroux	The cyclodextrins to discriminate at single sulfur atom the polysulfides by nanopore and design binders to improve batteries
12h15	Invited Conchi Ania	Advanced characterization of nanoporous materials: scanning hysteresis loops to explore pore connectivity
12h40	Lunch	
14h	Keynote Alexander V. Neimark	Advanced characterization of structural and adsorption properties of metal-organic frameworks
14h45	Invited Luis Mafra	Understanding CO ₂ sorption mechanisms in porous adsorbents via surface-enhanced NMR
15h10	Invited Tom Bennett	Synthesis, and characterisation of non-crystalline MOF structures
15h35	Pause	
16h05	Invited Ana Platero	Applications of pair distribution function analyses to non-ideal porous frameworks
16h30	Flash pres. Artem Kovalenko	Collapse and cavitation during the drying of water-saturated PDMS sponges with closed porosity
16h40	Flash pres. Antoine Tissot	Robust MOFs for applications in energy
16h50	Flash pres. Clio Parisi & Francisco Fernandes	Enter the biomimetic Matrix: shaping porous materials for 3D cell culture applications using ice
17h	Invited Timo Betz	Cancer cell invasion in porous collagen matrices
17h25	Invited Guillaume Charras	Living cells as poroelastic material
17h40	Pause	
17h50	Flash pres. Simona Mura	When drug nanocarriers miss their target: extracellular diffusion and cell uptake are not enough to be effective
18h	Flash pres. Ruxandra Gref	«Cage» nanoparticles to treat cancer and infections
18h10	Flash pres. Laurent Corte	Porous nanoparticle coatings for hydrogel-tissue adhesion
18h10	Closing first day	

Programme

Day 2

9h45	Opening	
10h	Keynote Yi Tao Long	Nanoconfinement controlled chemistry for single - molecule sensing
10h45	Invited Mathias Winterhalter	Selective transport in porous material: permeation across bacterial channel at single channel level
11h10	Pause	
11h40	Flash pres. Clemence Sicard	Synthesis and characterizations of bacteria and metal-organic frameworks based biohybrids
11h50	Flash pres. Daniel Grande	Design and multi-scale investigation of biporous bioinspired polymeric materials
12h	Flash pres. Elisa Bindini	In situ ellipsometry to assess the degradation of porous materials
12h10	Invited Camille Petit	CO ₂ photoreduction using porous amorphous catalysts
12h35	Lunch	
14h	Keynote Silvia Bordiga	Catalytic materials under investigation through the eye of a spectroscopist
14h45	Invited Tina Düren	Combining molecular simulation and machine learning: autonomous investigation of porous solids for adsorption applications
15h10	Pause	
15h40	Invited Thomas Bein	Optoelectronic processes in covalent organic frameworks
16h05	Invited Rob Ameloot	Direct lithography of metal-organic framework films
16h30	Flash pres. Qui Pham Xuan	Building responsive materials by assembling {Fe ₄ Co ₄ } switchable molecular cubes
16h40	Flash pres. Mohamed Nawfal Ghazzal	Tuning the electronic bandgap of Graphdiyne by H-susbtitution for optimal interfacial charge transfer and photocatalytic H ₂ generation
16h50	Flash pres. Anne Dolbecq & Caroline Mellot Draznieks	POM@MOF composites for CO ₂ reduction : combining solid state NMR, PDF and DFT calculations for rationalizing photocatalytic activities
17h	Flash pres. Véronique Balland	Reversible proton insertion in amorphous and anatase nanostructured TiO ₂ electrodes.
17h10	Flash pres. William Shepard	
18h20	Closing congress	



Invited



Robert Dominko

National Institute of Chemistry, Ljubljana, Slovenia

Bio sourced membranes as interlayers in Li batteries

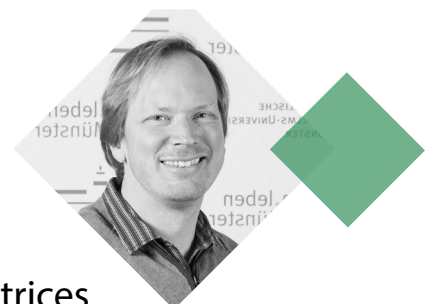
Biosourced materials represent a group of sustainable functional materials with low CO₂ footprint. Their versatility and enormous possibilities for modifications make them as potential candidates for different applications among the also in Li-ion batteries. In our recent work we applied a modified nanocrystalline cellulose as a protection interlayer for lithium metal.[1,2] Few micron thick layers of cellulose where interspace voids are filled with additives effectively prevent constant exposure of metallic lithium towards electrolyte and anisotropy of cellulose fibers stops dendrite growth. The beneficial influence of the protective layer based on cellulose composite was confirmed with long-term lithium stripping and deposition, long term cycling in carbonate and ether-based electrolytes, ex-situ focused ion-beam scanning electron microscope (FIB-SEM), operando ATR-IR spectroscopy and impedance spectroscopy. Even more controlled transport in Li-ion batteries can be achieved with application of membranes selective for certain species. Those made of solid materials excel in durability and integrity, however production of accurate and uniform pores is demanding, usually high selectivity is hard to meet. Biological pores on the other hand have the advantage of atomically determined structure, which is always the same. Many of them can achieve high selectivity with additional optimisation by using protein engineering. Inconveniently, they are found in nature in lipid bilayers, which are unstable what limits their use. Research activities leading to the application of the Lysozyme protein in Li-ion batteries will be discussed. [3]

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- [2] N. Pavlin, R. Dominko, Silylated cellulose based interfacial protective layer on a lithium surface, European patent 3 818 578 (WO 2020/007980).
- [3] S. Kolar, PhD disertation topic

Timo Betz

Institute of cell biology, ZMBE,
University of Münster, Germany



Cancer cell invasion in porous collagen matrices

The inside of living cells is filled with cytoplasm, a biphasic material consisting of a porous elastic solid meshwork (comprising the cytoskeleton, organelles, and macromolecules) bathed in an interstitial fluid called cytosol. As the cytoplasm is the largest part of the cell by volume, its rheology sets the rate at which cellular shape changes can occur. I will present experimental data showing that the cytoplasm behaves as a poroelastic material. We use mechanical, chemical, and genetic treatments to perturb the organisation of the cytoplasm to examine the dependency of cell rheology on porosity. Next, I will present experiments suggesting that pressure gradients induced in the cytoplasm can be sustained over several minutes thanks to the interplay between cytoplasmic poroelasticity and water flows across the membrane. Overall our data suggest that intracellular cytosolic flows and pressure gradients may play a much greater role than currently appreciated in cell rheology.



Camille Petit

Department of Chemical Engineering, Barrer Centre,
Imperial College London, UK

CO₂ photoreduction using porous amorphous catalysts

Reshaping our energy portfolio considering the sustainability of global energy resources is central to the European Energy Roadmap 2050. Hence, researchers need to identify efficient routes towards solar fuels production. Comparatively to H₂ evolution, CO₂ photoreduction has been poorly studied. Given the scope for CO₂ utilisation in a carbon-constrained future, there is an exciting opportunity to devote targeted research towards CO₂ photoreduction. Photocatalysis is one route towards CO₂ reduction. Yet, the design of a cost-effective, sustainable, efficient and robust photocatalyst remains a highly challenging task. To date, the majority of studies on CO₂ reduction photocatalyst focuses on crystalline and non-porous materials, with TiO₂ remaining the 40-year old benchmark in the field. Yet, porous amorphous materials can present interesting photocatalytic features. The high surface area allows one to favour access to catalytic sites, tune the strength of adsorption/desorption of reactants/products and possibly control electronic transfer mechanisms. Scaling up amorphous materials synthesis can be easier than for crystalline materials. Herein, we will discuss our recent work towards the development of CO₂ photoreduction catalysts that present both a porous and an amorphous character. We will highlight in particular our studies on boron nitride and hypercrosslinked polymers, two types of materials that do not involve any rare-earth metals. For both types, we show that the selective conversion of CO₂ into CO is possible under both UV and visible light. Using analytical and spectroscopic tools, we are starting to understand the mechanisms of reaction of these materials.

Luis Mafra

Department of Chemistry,
University of Aveiro, Portugal.



Understanding CO₂ sorption mechanisms in porous adsorbents via surface-enhanced NMR

The nature of CO₂ species interacting with porous surfaces determines the gas sorption capacity/kinetics, selectivity and cyclic stability of a given adsorbent material. However, an atomic-level understanding of the CO₂ sorption process remains elusive, hindering our ability to design improved sorbents. The lack of advanced spectroscopic studies, tailored to elucidate the structure of adsorbed gas species, has also been a major bottleneck for further progresses in understanding the physical chemistry of gas-solid interfaces. Adapting spectroscopic tools to the study of confined gas species, interacting with porous surfaces, is also not trivial. This presentation shows that solid-state (ss) NMR spectroscopy is a unique bulk or surface site-selective technique to study material surfaces of amorphous porous CO₂-adsorbents. Strategies combining ssNMR and computational methods to study CO₂ speciation, under dry and wet conditions, are showcased.



Rob Ameloot

KU Leuven Belgium

Direct lithography of metal-organic framework films

Metal-organic frameworks (MOFs) offer disruptive potential in micro- and optoelectronics because of the unique properties of these microporous materials. Nanoscale patterning is a fundamental step in the implementation of MOFs in miniaturized solid-state devices. Conventional MOF patterning methods suffer from low resolution and poorly defined pattern edges. In this case study, the resist-free, direct X-ray and electron-beam lithography of MOFs will be demonstrated. This process avoids etching damage and contamination and leaves the porosity and crystallinity of the patterned MOFs intact. The resulting high-quality patterns have excellent sub-50-nm resolution, and approach the mesopore regime.

Chris McMinn

Department of Engineering Science
University of Oxford, UK



Fluid-fluid phase separation in a soft porous medium

The interactions of two fluids within a porous medium depend strongly on flow conditions, wettability, and the structure of the pore space. At the pore scale, these interactions are characterised by the formation of wetting films that coat solid surfaces and occupy corners and throats, and the formation of non-wetting blobs that occupy larger pore bodies. The invasion of non-wetting blobs into narrow throats is energetically unfavorable, but it can be forced with a sufficiently high pressure gradient. A soft porous medium is one in which the pore structure can deform in response to the flow. The most striking feature of two-fluid-phase flow in a soft porous medium is the tendency of the non-wetting phase to enlarge the pore space by pushing the solid grains apart, to the point of forming macroscopic cavities in the medium. These cavities can be much larger than the pore scale, and they form spontaneously when the energetic benefit of reducing the Laplace pressure exceeds the energetic cost of deforming the solid skeleton. Here, we consider this process through the lens of phase separation, where a non-wetting phase separates (or not) from a fluid-fluid-solid mixture. Informed by the thermodynamics and large-deformation poromechanics of this system, we construct a phase-field model in which two immiscible fluids interact with a poroelastic solid skeleton. Our model captures the competing effects of elasticity, confinement, flow, and fluid-fluid-solid interactions. We then use our model to consider an initial distribution of non-wetting fluid in the pore space that separates into multiple cavities. We identify the key parameters that control phase separation, the conditions that favor the formation of cavities, and the characteristic size of the resulting cavities. We complement this analysis with experimental observations. Our results have implications for a wide variety of natural and industrial systems, such as the nucleation and growth of gas bubbles in lake beds and waste ponds.



Jan Carmeliet

Chair of Building Physics, ETHZ, Switzerland

Anomalous water transport in multiscale porous materials like textiles

Textiles are ubiquitous as clothing, in medical, sport or hygienic care, but also in engineering or architecture. The control of liquid spread in these materials is often crucial or desirable, such as e.g. moisture management in functional clothing or durability of fiber reinforced materials. Fast X-ray tomographic microscopy and Neutron radiography are used to monitor the imbibition process in yarns at micrometer and centimeter scale, respectively. Observed is a step-wise water uptake process characterized by fast pore filling events of long and narrow pores in the order of seconds and long waiting times between filling events up to several minutes. This step-wise dynamics results in an uptake behavior not following the square root behavior as described by Washburn's law. The step-wise dynamics are analyzed in terms of the balance between free energy and viscous dissipation, showing waiting times are corresponding to quasi-stable water configurations of almost vanishing free energy gradient. A pore network model is developed based on the typical pore network topology of yarns and waiting time distributions as observed at micron scale. This network model is upscaled to millimeter scale and validated with the Neutron measurements. The network model allows to analyse in detail the interplay of pore scale processes and pore network topology at lower scales and their impact on experimentally observed processes at macroscale.

Guillaume Charras

Centre for Nanotechnology and Department of Cell and Developmental Biology, University College London, UK.

Living cells as poroelastic material

The inside of living cells is filled with cytoplasm, a biphasic material consisting of a porous elastic solid meshwork (comprising the cytoskeleton, organelles, and macromolecules) bathed in an interstitial fluid called cytosol. As the cytoplasm is the largest part of the cell by volume, its rheology sets the rate at which cellular shape changes can occur. I will present experimental data showing that the cytoplasm behaves as a poroelastic material. We use mechanical, chemical, and genetic treatments to perturb the organisation of the cytoplasm to examine the dependency of cell rheology on porosity. Next, I will present experiments suggesting that pressure gradients induced in the cytoplasm can be sustained over several minutes thanks to the interplay between cytoplasmic poroelasticity and water flows across the membrane. Overall our data suggest that intracellular cytosolic flows and pressure gradients may play a much greater role than currently appreciated in cell rheology.



Mathias Winterhalter

Jacobs University Bremen, Germany

Selective transport in porous material: permeation across bacterial channel at single channel level

The outer cell wall in Gram-negative bacteria is a sophisticated filter to reject cell toxic substance but allow nutrient to enter. The key building block are membrane channels known as porins. Our team is interested in quantifying the flux across these nanopores and to elucidate what parameter in addition to size influence the transport. We give a short overview how to measure the fluxes and what are the typical rates.

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Tom Bennett

Department of Materials science and Metallurgy of Cambridge, UK

Synthesis, and characterisation of non-crystalline MOF structures

Porous 'hybrid' materials such as MOFs consist of both inorganic and organic components, and contain regions of empty space into which guest molecules can be selectively adsorbed and sometimes chemically transformed. A variety of applications have arisen, including e.g. clean air and water production, drug delivery and the prevention of fruit over-ripening. They are often ordered (crystalline) solids, and order—or uniformity—is frequently held to be advantageous, or even pivotal, to our ability to engineer useful properties in a rational way.

Glasses on the otherhand are 'frozen liquids', which open our eyes to the world, and connect us together. They allow us to store and retrieve digital memories, display information and enable life-saving surgical interventions. Their attractive physical properties, alongside those of non-glassy amorphous solids, are heavily employed across the materials spectrum in strikingly diverse applications such as display technologies, photovoltaics, coatings and pharmaceutical packing. It is surprising that the interdisciplinary area between amorphous materials and MOFs is almost totally neglected. This is despite the massive opportunities arising from the ability to alter existing glass chemistries with a given set of chemical, and physical properties. Examples are given of their formation, and potential uses and interests of the non-crystalline state.



Tina Düren

Department of Chemical Engineering,
University of Bath, UK

Combining molecular simulation and machine learning: autonomous investigation of porous solids for adsorption applications

With a sheer infinite number of hypothetical and already synthesised MOFs and COFs to choose from, molecular simulations are invaluable for identifying promising candidates for applications such as gas storage or advanced separations. They are significantly cheaper than experimental synthetic approaches, allowing many materials to be assessed in quick succession. Numerous large-scale screenings of porous materials have been conducted, assessing the performance of hundreds of thousands of structures using molecular simulations. However, they are expensive and can lack accuracy, often relying on finding a compromise between computational costs and calculating the property of interest for all structures precisely. Furthermore, this brute-force approach becomes impractical when considering mixtures of guest molecules, complex guest molecules, and different experimental conditions.

To further reduce the time taken for materials discovery, some research groups have trained machine learning models on the screening data sets, with varying results. A core problem is the focus on traditional machine-learning prediction, where a model is first trained and then used to estimate properties of interest for all structures in the data set. It is only after a large number of simulations have been conducted that the model can be used to identify the top performing new materials for the application of interest.

Combining Bayesian optimisation and molecular simulation we have developed a new approach, which we call the Autonomous Materials Investigator (AMI) [1], which allows us to identify the top performing materials of a database without having to calculate the property of interest for 10,000s of individual structures. One of the core attractions of this new methodology is that our model can make recommendations based on limited information, updating itself in-situ from molecular simulation of performance for a given application.

Using the hCOF (hypothetical covalent organic frameworks) [2] and the hMOF (hypothetical metal-organic frameworks) [3] databases, we demonstrate the AMI's impressive efficiency. For example, the AMI identifies 90 of the top 100 performing structures from 69,480 hCOF structures with less than 500 calculations for methane storage. This performance allows us to perform screening for more computationally expensive applications. Moreover, our method can also integrate experimental inputs in addition to simulations to allow for further aspects of the materials to be considered during screening or be adapted to assess materials for materials performance targets beyond adsorption.

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Acknowledgements

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Thomas Bein

Department of Chemistry, University of Munich, Germany

Optoelectronic processes in covalent organic frameworks

Photoactive molecular building blocks can be spatially integrated into the crystalline lattice of covalent organic frameworks (COFs), allowing us to create models for organic bulk heterojunctions, chemical sensors and porous electrodes for photoelectrochemical systems. In this presentation, we will address means of controlling the morphology and packing order of COFs in thin films (1) and with spatially locked-in building blocks.(2)

We will discuss different strategies aimed at creating electroactive networks capable of light-induced charge transfer. For example, we have developed a COF containing stacked thienothiophene-based building blocks acting as electron donors with a 3 nm open pore system, which showed light-induced charge transfer to an intercalated fullerene acceptor phase.(3) Contrasting this approach, we have designed a COF integrated heterojunction consisting of alternating columns of stacked donor and acceptor molecules, promoting the photo-induced generation of mobile charge carriers inside the COF network.(4) Additional synthetic efforts have led to several COFs integrating extended chromophores capable of efficient harvesting of visible and near infrared light, for example (5). Extending newly developed thin film growth methodology to a solvent-stable oriented 2D COF photoabsorber structure, we have recently established the capability of COF films to serve in photoelectrochemical water splitting systems.(6) The detailed mechanism of excited state dynamics in light-harvesting conjugated COFs has been revealed by means of transient absorption spectroscopy.(7) Many optoelectronic applications of COFs depend on significant electrical conductivity. Here, Wurster-type structural motifs are attractive building blocks for imparting high conductivity in the corresponding COFs.(8) Finally, COF films can also act as ultrafast solvatochromic chemical sensors (9) and show very efficient electrochromic response.(10) The great structural diversity and morphological precision that can be achieved with COFs make these materials intriguing model systems for organic optoelectronic materials.

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Conchi Ania

CEMHTI, CNRS Univ. Orleans, France

Advanced characterization of nanoporous materials: scanning hysteresis loops to explore pore connectivity

The analysis of gas adsorption/desorption isotherms is a valuable tool to characterize and comprehend the porous features of materials with tailor-made nanopore architectures in the micro- and mesoporous range. Various methods (i.e., Dubinin-Radushkevich, BJH, t-plot, density functional, molecular simulation) have been extensively used for this purpose, allowing the determination of the apparent surface areas, pore volumes and pore size distributions [1]. However, while the characterization of microporous materials is fairly well established, the assessment of the pore structure for mesoporous materials is still a challenge [2-4]. In this context, the analysis of the hysteresis loops of the gas adsorption isotherms by means of advanced experimental procedures such a hysteresis scanning becomes an interesting tool for this purpose. In this work we have analyzed the nanoporosity of mesoporous carbons by recording the gas adsorption isotherms of various probes (e.g. N₂, Ar, CO₂), performing scanning curves of the hysteresis loops and applying different models for data interpretation. A special emphasis will be paid for unravelling the connectivity of the mesopore network in the studied materials

Acknowledgements. The authors thank the financial support of the H2020 through a Consolidator Grant (648161).
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- [4] T. Nguyen, D.D. Do, D. Nicholson, J. Phys. Chem. B 115, 12160-726 (2011).

Ana Platero

Autonomous University of Madrid, Spain



Applications of pair distribution function analyses to Non-Ideal porous

Covalent- and Metal-Organic Frameworks (COF and MOF), composed of molecular components connected to give porous architectures, have demonstrated to be unexpectedly dynamic. Porous framework materials have been commonly regarded as static frameworks, mostly driven by a conventional understanding of crystallinity. In this talk we will discuss how this idea is incomplete and needs to be rethought. What is the real structure of a MOF or a COF under working conditions? How dynamic these materials are? Which is the role of local distortions and rearrangements in the ultimate properties of these materials? Using advanced X-ray scattering characterization tools we can look at the atomic structure of materials regardless their degree of crystallinity, providing a better understanding of these materials under conditions relevant for applications.

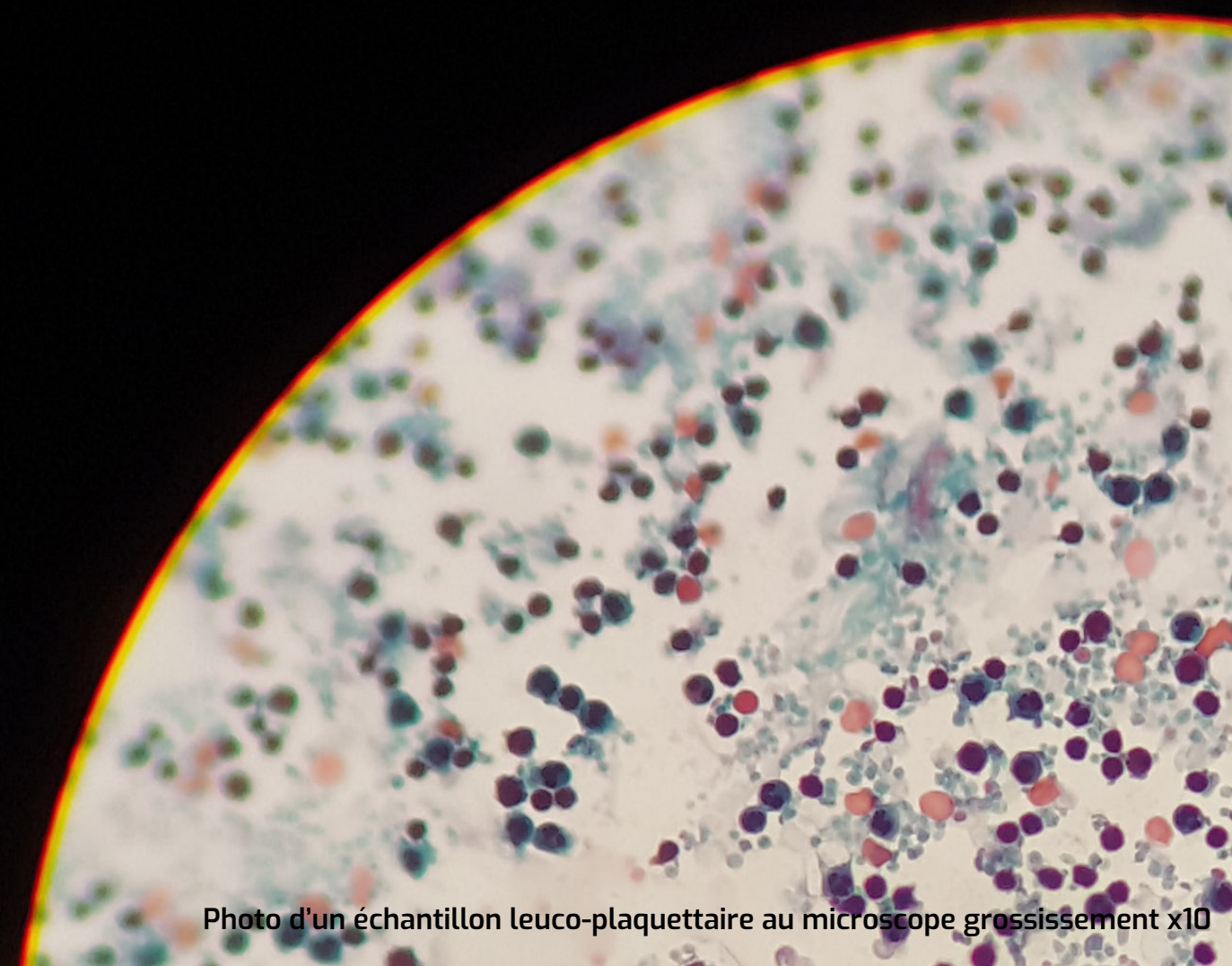


Photo d'un échantillon leuco-plaquettaire au microscope grossissement x10

Flash presentations



Clément Campillo

University of Evry, France

Mechanics of micropatterned cancer cells by AFM

The mechanical properties of living cells reflect their physiological and pathological states. In particular, cancer cells are generally softer than their healthy counterparts and tumors harder than normal tissue. These mechanical properties, determined largely by the cytoskeleton and the plasma membrane, govern the processes of migration, division or cell spreading. Nevertheless, studying cellular mechanics and being able to use it as a diagnostic tool is a challenge because of the complexity of the structure and organization of the cells. Therefore, we use adhesive micro patterns to measure in a standardized way the mechanical properties of the cells by AFM in relation to their metastatic potential. With the micro patterns, all the cells considered then have the same geometry, the same architecture and the same microenvironment, thus reducing inter and intra-cellular variability. We culture cancer cells on micro-patterns and use an AFM mode that allows us to obtain their elasticity and morphology from indentation curves with a high resolution, typically several hundreds of measurements per cell. We then analyze these data to extract the averaged cell morphology and elasticity map and compare different populations of cells representing various stages of cancer progression.

Abdelghani Oukhaled

CY Cergy Paris University, CNRS, LAMBE, France



On single-molecule protein sequencing through nanopores: challenges and opportunities

My talk focuses on the concept of protein sequencing through nanopores at single molecule level. I discuss the main works done in this direction, in particular those recently done in our laboratory. Perspectives will be proposed and discussed.



Artem Kovalenko

ESPCI Paris, Sorbonne University, PSL University, CNRS, France

Collapse and cavitation during the drying of water-saturated PDMS sponges with closed porosity

Soft elastomer foams are promising materials for different applications [1], including sensing, soft actuation or acoustic metamaterials. However, a major scientific deadlock for the fabrication of these materials is the control over the pore size : it is still a challenge to reliably make pores below the 1 μm which would enable metamaterials with micro-architected or gradient porous structures [2]. Indeed, at this «colloidal» lengthscale, the classic foam polymerization methods are poorly controllable and more innovative «template» methods are required. In this work [3], we use water/polydimethylsiloxane (PDMS) emulsions to fabricate soft macroporous samples with average pore diameters ranging from 10 to 300 μm . We focus on drying of these materials with closed porosity which is possible only via the diffusion across the PDMS. We demonstrate the existence of a critical pore diameter under which the drying leads to the irreversible pore collapse while pores with larger diameters reopen via cavitation. This phenomenon opens new routes to the tailoring of porous structure of soft sponges.

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3. Nguyen et al. Soft Matter 2020. <https://doi.org/10.1039/D0SM00932F>.

Antoine Tissot

Paris porous materials institute, France



Robust MOFs for applications in energy

Metal-Organic Frameworks (MOFs) are fascinating porous hybrid solids with potential applications in the field of health, energy and environment. However, the development of chemically robust MOFs is a prerequisite for their integration into real devices. In this contribution, I will present our recent efforts dedicated to the synthesis and structural characterization of chemically stable Zr(IV) and Ti(IV)-based MOFs, along their use as porous matrix to immobilize catalytically active species for energy-related reactions such as carbon dioxide methanation¹ and dehydrogenation of formic acid².

[1] S. Wang et al. Chem 2020, 6, 3409.

[2] S. Wang et al. Matter 2021, 4, 182.



Nathalie Jarroux

Paris-Sarclay University, CNRS, LAMBE, France

The cyclodextrins to discriminate at single sulfur atom the polysulfides by nanopore and design binders to improve batteries

In the last decades, research efforts on batteries have been focused on increasing of energy density and durability. Life sciences have inspired the development of smart batteries embedded with self-healing functionalities¹ among their components (e.g., electrode, separators, electrolyte). This calls for supramolecular interactions which represent a useful tool to either regulate species migration at the electrolyte/membrane interface² or restore electrode conductivity³. In this work we focus on cyclodextrins (CDs), which are bio-sourced cage molecules that can give reversible supramolecular interactions with a guest molecule.

On the one hand, we successfully exploited the selective host-guest interaction of CDs to trap polysulfides and discriminate them by nanopore with a single sulfur atom resolution. This approach opens the way to the design of powerful sensors for Li-S batteries electrolytes based on the nanopore technology⁴.

On the other hand, we applied this host-guest interaction at the macromolecular scale by synthesizing polyrotaxanes (PRs) based on CDs and poly(ethylene oxide) (PEO) while controlling their structural parameters (polymer length, number of threaded CDs...). The PRs are crosslinked with poly(acrylic acid) and used as Si anode binders. Since CDs can freely move along the polymer chain, pulley effect are giving to these materials which lead to new routes of accommodating the volume change of the Si anode and improving the cycling performances of the battery.

1. Vegge, T., Tarascon, J. M., & Edström, K., Advanced Energy Materials, 2021, 2100362

2. Zhao Y., Zhang Y., Sun H., Dong X., Cao J., Wang L., Xu Y., Ren J., Hwang Y., Son I. H., Huang X., Wang Y. Peng H., Angew. Chem. Int. Ed., 2016, 55, 14384-14388

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William Shepard

Synchrotron Soleil, Gif-sur-Yvette, France



Simona Mura

Galien Paris-Sarclay Institute, France

When drug nanocarriers miss their target: extracellular diffusion and cell uptake are not enough to be effective

Biocompatible nanoscale iron carboxylate metal organic frameworks (nanoMOFs) already demonstrated their ability to efficiently deliver various therapeutic molecules. The versatility of the synthetic methods and functionalization strategies could further improve their drug carrier potential. However, in oncology, preclinical evaluation still suffers from the lack of relevant models able to mimic the heterogeneity and the microenvironment of human tumors. This may impact the significance of the preclinical data, hindering the clinical translation and drug development process. Motivated by this hurdle, a 3D lung tumor model is herein developed to investigate nanoMOFs, as bare nanoparticles or coated with polyethylene glycol. Loading with doxorubicin, as a model drug, allows investigating their penetration capacity and efficacy in the 3D tumor nodule. NanoMOFs carry a large cargo, can diffuse efficiently within the tumor and are capable of significant intracellular penetration. Nevertheless, they prove therapeutically ineffective because the loaded drug does not reach the nucleus, the doxorubicin sub-cellular target. These results question the in vivo evaluation and call for further optimization to achieve successful drug delivery.

Mohamed Nawfal Ghazzal

Institute of physics chemistry
Orsay, France



Tuning the electronic bandgap of Graphdiyne by H-substitution for optimal interfacial charge transfer and photocatalytic H₂ generation

Solar water splitting into hydrogen is one of the promising means for dealing with energy shortage and environmental problems. H-substituted graphdiyne (H-GDY), for the first time, is employed to fabricate a heterojunction with P25 to improve the photocatalytic activity. The obtained TiO₂/H-GDY heterojunctions were characterized by XRD, EDX, TEM, XPS and UV-vis spectrums to ascertain the structure and electronic properties of the composites. Enhanced photocatalytic properties were demonstrated for the as-prepared samples. The influence of the H-GDY content on the photocatalytic activity was investigated and all the samples showed enhanced photocatalytic activity. The amount of hydrogen by the optimized heterojunctions was ~370 mmol after 6 hours test, much higher than that of pristine P25. Such enhancement was ascribed to the H-GDY/P25 heterojunction structure, which can simultaneously improve the absorption of visible light and facilitate the photo-excited electron-hole separation during the photocatalytic process. This work opens new perspectives for application of H-GDY in photocatalytic field.



Clémence Sicard

Lavoisier Institute of Versailles, France

Synthesis and characterizations of bacteria and metal-organic frameworks based biohybrids

Micro-organisms have developed remarkable mechanisms to handle high concentrations of organic pollutants in their environment. However, the use of microorganisms as biocatalytic entities often requires immobilisation within solid-supports, in order to provide protection, controlled environment, recyclability, recovery and to minimise leaching of exogenous strains. Compared to enzymes, preservation of cellular activity within solid hosts is more challenging but they give access to multi-cascade catalysis pathways and also spare from any complicated and time-consuming processes required for enzyme production, isolation and purification. Metal-Organic Frameworks (MOFs) has recently arise as an alternative and promising strategy to answer the limitations of traditional immobilization matrices, resulting in the design of novel functional biomaterials with promising properties.[1] We will present our latest findings on the synthesis and characterization of MOFs-based living materials.

[1] (a) K. Liang et al, Adv. Mater. 2016, 28, 7910; (b) E. Gkaniatsou et al Mater. Horiz. 2017, 4, 55; (c) W. Liang et al Chem. Rev. 2021, 1077

Xuan Qui Pham

Parisian Institute of Molecular Chemistry,
Sorbonne University, France



Building responsive materials by assembling {Fe₄Co₄} switchable molecular cubes

Responsive materials that can answer to chemical or physical external stimuli offer numerous prospects in material science. Here, we elaborated a two-step synthetic approach that allows incorporating molecular cubic switches into a polymeric material. Firstly, a preformed half-capped, Cs⁺-templated {Fe₄Co₄} cyanido-polymetallic cubic unit ("pro-cube") is obtained and proven to be stable in solution, as demonstrated by paramagnetic NMR. Secondly, the reaction of the pro-cube with a ditopic scorpionate ligand enables the precipitation of a polymeric network containing the cubic unit. Furthermore, the adequately chosen ditopic ligand that coordinates the Co ions of the pro-cube allows us to preserve the switchable properties of the cubic unit. Indeed, the magnetic properties of the polymeric material compare well with those of the molecular cubic model that is obtained by reacting a non-bridging scorpionate ligand, and that was prepared as a reference. Both the polymeric material and the molecular model cube show a thermally-induced metal-metal electron transfer near room temperature. Interestingly, the magnetic state of the polymeric material is shown to depend on its hydration state, indicating its capability to act as a chemo-sensor.



Anne Dolbecq

Lavoisier Institute of Versailles,
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Caroline Mellot Draznieks

Biological process chemistry laboratory,
Sorbonne University, France



POM@MOF composites for boosting CO₂ reduction : combining solid state NMR, PDF and DFT calculations for rationalizing photocatalytic activities

In the current energetic crisis, the photoreduction of CO₂ to energy-dense organic molecules (CO, HCOOH, etc.) under visible-light illumination is considered as a green and sustainable however challenging strategy. The heterogenization of molecular catalysts for CO₂ reduction into Metal-Organic Frameworks (MOFs) is an attractive strategy which combines the advantages of homogeneous catalysis (modulation of activity via structural modification) and heterogeneous catalysis (easy recovery, thin films processability) [1]. In this context, a POM@MOF composite catalyst for CO₂ reduction, namely (POM,Cp^{*}Rh)@UiO-67, was synthesized by co-immobilizing a molecular Rh-catalyst for CO₂ reduction and a polyoxometalate (POM) in the UiO-67 type MOF. In photocatalytic conditions, the formate production was doubled when compared with that observed using the POM-free Cp^{*}Rh@UiO-67 catalyst [2] and reached TONs as high as 175 when prepared as thin films, showing the beneficial influence of the POM on CO₂RR. We will show in this presentation how the combination of several characterization techniques (XRD, IR, 31P and 13C NMR, PDF) allowed to confirm the integrity of the whole (POM,Cp^{*}Rh@MOF) composite over the catalytic event. The combination Monte Carlo and DFT calculations with ssNMR revealed two possible locations of the POM in the octahedral cavities of the MOF, while elucidating the role of the POM in the CO₂ reduction reaction mechanism [3].

[1] P. Mialane et al. Chem. Soc. Rev. 2021, 50, 6152.

[2] M.B. Chambers et al. ChemSusChem. 2015, 8, 603-608.

[3] Y. Benseghir et al. J. Am. Chem. Soc. 2020, 142, 9428.



Daniel Grande

Institute of Chemistry and Materials, Paris-East, France

Design and multi-scale investigation of biporous bioinspired polymeric materials

Devising model polymeric porous media that exhibit the specific properties of wood during imbibition, drying and filtration constitutes an interesting challenge. The main objectives of this work consist in reinforcing the understanding of these physical phenomena and in providing new porous structures with original properties. The novelty of our approach lies in the use of tailor-made biporous bioinspired materials, which intends to reproduce several complex aspects of the wood structure at the origin of such physical processes. In this context, two porogenic agents were employed: a porogenic solvent to generate the nanopores and Nylon® threads to form the tubular macropores. To this purpose, bio-based monomers arising from lignin were synthesized to chemically mimic wood structure: syringyl methacrylate for hardwood, guaiacyl methacrylate and vanillin methacrylate (VMA) for softwood. Different structural parameters were shown to clearly have an impact in the porous features of the nanoporous network via mercury intrusion porosimetry, namely the porogenic solvent polarity, the monomer nature and the solvent/comonomers volume ratio. Moreover, scanning electron microscopy and X-ray microtomography were used to verify the morphology of the macropores. Finally, transfer properties of such anisotropic biporous materials were investigated. Permeability and imbibition measurements were carried out with 2-hydroxyethyl methacrylate-based materials as the corresponding polymer was extensively studied in our group. These results were then compared with those obtained from VMA-based materials.

Ruxandra Gref

Orsay Institute of Molecular Sciences, France



«Cage» nanoparticles to treat cancer and infections

Treating intracellular infections is particularly challenging, requiring the drugs to bypass biological barriers such as cellular membranes to reach the pathogens in their niches. Many drugs poorly penetrate inside cells, necessitating to increase the administered doses which in turn can lead to unwanted side-effects and drug resistance. In this context, engineered nanoparticles (NPs) were used as "Trojan horses" to carry an active drug combination inside infected cells. "Cage" NPs possess internal interconnected compartments prone to load high drug payloads. Interestingly, some NPs were found to co-localize with the pathogens. Advantageously, they degraded inside the cells to release the drug cargo, eradicating the pathogens. Moreover, certain engineered NPs are also endowed with their own antibacterial properties. These results pave the way toward the design of "all-in-one" nanocarriers in which both the NPs and the loaded drugs play a role in fighting infections.



Clio Parisi

CRB Lariboisière- LCMCP, France

Francisco Fernandes

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Enter the biomimetic Matrix: shaping porous materials for 3D cell culture applications using ice

3D cell culture methods keep gaining momentum as more appropriate biomimetic substrates compared to conventional (2D) culture, since they present higher physiological relevance. 3D in vitro models mimicking the extracellular matrix (ECM) in terms of composition, architecture, and mechanical properties are needed in order to study complex pathologies, such as cancer. Despite the large spectrum of fabrication strategies, obtaining the appropriate macroporosity while avoiding cytotoxicity related to inherent process limitations remains a critical issue.¹ To tackle these constraints, ice-templating as a biofabrication technique enables the creation of strictly oriented pores under non-denaturing conditions.² In particular, highly concentrated type 1 collagen solutions can be converted to macroporous fibrillar scaffolds, with precisely defined topological, mechanical, and biological cues, suitable for 3D cell culture applications.³ Porosity is highlighted as a key factor to promote cell migration in a 3D environment while the induced self-assembly of ice-templated collagen provides an invaluable approach to obtain macroporous scaffolds displaying the ultrastructural features of the ECM

¹ Parisi C, Qin K, and Fernandes FM, Colonization vs. encapsulation in cell-laden materials design: porosity and process biocompatibility determine cellularization pathways, Phil. Trans. R. Soc., 2021, accepted, in production

² Qin K, Parisi C, and Fernandes FM, Recent advances in ice templating: from biomimetic composites to cell culture scaffolds and tissue engineering, J Mater Chem B., 2021, 9(4):889-907, doi: 10.1039/d0tb02506b

³ Rieu C, Parisi C, Mosser G, Haye B, Coradin T, Fernandes FM, and Trichet L, Topotactic Fibrillogenesis of Freeze-Cast Micro-ridged Collagen Scaffolds for 3D Cell Culture, ACS Appl Mater Interfaces, 2019, 11(16):14672-14683. doi : 10.1021/acsami.9b03219



Elisa Bindini

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In situ ellipsometry to assess the degradation of porous materials

Ellipsometry is a fast, non-destructive technique to obtain the optical properties of a sample material through the reflected light waves. The technique measures a relative change in polarization and is therefore not dependent on absolute light intensity, which makes ellipsometric measurement very accurate and reproducible. The optical properties of the studied materials can be modeled choosing the appropriate mathematical functions, and in the case of porous materials effective medium approximation theories (EMA) can be used. With EMAs the dielectric function of the material can be calculated based on a mix of two or more known dielectric functions, for example the one of the material inside the pores and the one of the matrix material. In this way, porosity values can be quickly obtained. The interesting assets of ellipsometry to study degradation or corrosion is that it is a fast measurement method and it can be performed in a liquid environment as long as the media is transparent. Therefore, it can be employed to follow the material evolution in situ, analyzing the change in its optical properties and its thickness. In studies concerning porous materials the technique is particularly useful because it can follow in real time the porosity evolution when the material is exposed to a target atmosphere, liquid or flow. We used this method to monitor the degradation kinetics of mesoporous silica thin films in buffer solutions at 37 °C, shedding light on some unanswered questions regarding the use of mesoporous silica carriers for drug delivery purposes.

Laurent Corte

ESPCI Paris, France



Porous nanoparticle coatings for hydrogel-tissue adhesion

The fixation of hydrogels to soft biological tissues is of outmost interest for numbers of biomedical applications but it is a highly challenging task due to the fragile and wet nature of both hydrogels and tissues. Inspired by the pioneering works by Leibler and coworkers, we investigate here how tissue-hydrogel adhesion can be created using particles that bridge the interface by adsorbing on both gels and tissues. As an example, for a 5 min contact on liver tissues, a 3 to 4 fold increase in adhesion energy was obtained by simply coating dry PEG membranes with aggregates of silica or iron-oxide nanoparticles. Ex vivo and in vivo experiments show how adhesion depends on the contact parameters, nanoparticle size, surface and porosity as well as on the hydration of tissues. We find that in the presence of blood, the particle bridging effect combined to the procoagulant properties of silica nanoparticles provide a way to enhance the adhesion strength by inducing the rapid formation of a clot at the interface. These results and methods shed a new light on the design of predictive bioadhesion tests and on the strategies to control the fixation and biointegration of hydrogel based-devices.



Véronique Balland

Molecular electrochemistry laboratory,
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Reversible proton insertion in amorphous and anatase nanostructured TiO₂ electrodes.

The increase in the share of renewable and intermittent energies in the energy mix requires the implementation of energy storage devices at different scales that meet demanding criteria of economic and ecological sustainability. This is currently motivating the development of rechargeable batteries operating in mild aqueous conditions, which combine high conductivity, high safety and low cost, particularly the one based on an abundant charge carrier alternative to lithium ions. In this context, it is worth noting that H⁺ as charge carrier received little attention, despite its small size facilitating rapid diffusion with a minimum of steric constraints.

Here, we present a systematic analysis of the morphology and electrochemical charge storage properties of nanostructured amorphous and anatase TiO₂ electrodes in a mild aqueous buffered electrolyte. We demonstrate that both materials allow for reversible bulk proton insertion up to a maximal reversible gravimetric capacity of 150 mA·h·g⁻¹. We also show that the material crystallinity governs the energetics of the charge storage process, modelled by opposite short-range interactions in both phases, but has little effect on the interfacial charge-transfer rate as well as on the proton apparent diffusion coefficient, which is found one order of magnitude higher than that of Li⁺ in the same material. Finally, with both TiO₂ electrodes, reversible proton insertion allows to benefit from a gravimetric capacity as high as 95 mA·h·g⁻¹ at a high rate of 11 A·g⁻¹, outperforming the performances achieved with layered titanate films.



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Louis Flamencourt
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