ED182
PhD students' Congress
2026 edition

Program of the day

8:40 - 9:00		PhD's students welcoming - Registration	
9:00 - 9:05		Introduction words : S.Colis	
9:05 - 9:10	Sponsor segment	SPIE	S. Stefan
9:10 - 9:15		GFP	L. Biniek
9:15 - 9:20		Qmat	G. Weick
9:20 - 9:25		PUIA	F. Wasem-Klein
9:25 - 9:40	First oral session (J. Kapp)	Limitations to Cooling in Thermoelectric Nanodevices	J. Marty-Bazan
9:40 - 9:55		Development and industrial integration of PEDOT-based electrically conductive thermoplastic composites for plastronics and new generation connectors	Y. Venet
9:55- 10:10		Ab initio calculated magnetic coupling between magnetic nanoparticles on graphene	T. Robert
10:10 - 10:25		Electron-Hole Plasma/Liquid in suspended monolayer MoS2	S. Shetty
10:25 - 10:40		Fast Atom Diffraction through 2D Surface	P. Guichard
10:40 - 11:20		Coffee / tea break + poster session	
11:20 - 12:00	Invited speaker (V. Bouylout)	From lab to industry	F. Lallemand
12:00-13:00		Lunch	
13:00 - 13:10		Group photo	
13:15 - 13:30	Second oral session (A.Hoppenot)	Unveiling galaxies with AI: Deep Learning detection of neutral hydrogen in massive radio data	A. Anthore
13:30 - 13:45		To Cosmic Webs Through Neural Nets: 3D density field reconstruction from discrete tracers	G. Aichele
13:45 - 14:00		Unusual Non-linear Effects in Asymmetric Catalysis	J. El Khoury
14:00 - 14:15		Comprehensive TEM/STEM Analysis of High-Entropy Alloy Nanoparticles	N. Zhamantay
14:15 - 14:30		Quinoline based luminescent imidazolium salts as vectors for gene therapy	J. Kapp
14:30 - 15:35		Coffee / tea break + poster session // jury deliberation	
15:35 - 15:45		Closing words : M. Brinkmann	
15:45 - 16:00		Awards ceremony + final discussions	

QMat QUANTUM SCIENCE AND NANOMATERIALS

Fondation Jean-Marie Lehn

FRMNGE Fédération de Recherche Matériaux et Nanosciences du Grand Est

SPIE.

J. Marty-Bazan : Limitations to Cooling in Thermoelectric Nanodevices

Thermoelectric effects at the nanoscale offer promising routes for energy conversion and cooling in small electronic devices. In quantum coherent systems, where electrons propagate without losing phase information, energy dissipation mainly occurs outside the nanoscale conductor and affects the electronic reservoirs to which it is connected. Recent work by our team has revealed an asymmetry in energy dissipation between reservoirs under an applied voltage. In this work, we extend this analysis to finite temperatures by introducing a thermal gradient across the system, thereby coupling electrical and thermal transport. We focus in particular on the power dissipated in one reservoir and investigate the conditions under which it can be cooled by a thermoelectric effect. By analyzing the competition between electrical and thermal driving forces, we determine the minimal temperature that this reservoir can reach. Although this study is ongoing, these results highlight fundamental physical limits to thermoelectric cooling in quantum coherent devices that may be relevant for applications such as the cooling of solid-state qubits.

Y. Venet : Development and industrial integration of PEDOT-based electrically conductive thermoplastic composites for plastronics and new generation connectors

As copper reserves are increasingly running out, electrically conductive thermoplastic composites become of great interest. A recent strategy to fabricate such materials consists in the polymerization of PEDOT particles, an intrinsically conductive polymer, and their use as fillers into a thermoplastic matrix (PEO) through twin-screw extrusion [1]. The obtained composite exhibited conductivity up to 12 S.cm-1 , way higher than commercial equivalents using carbon-based fillers typically reaching 10-2 S.cm-1 [2], [3]. While continuing this work, results showed the possibility to transform it through several processes such as injection molding, overmolding and 3D printing, and its relevance for electronics was proved by designing demonstrators, arousing the interest of a firm. However, the material's high filler rate and its low compatibility with industrial context, among others, remain a major barrier. Such problems will be tackled by optimizing the composite's formulation (matrix, filler dispersion…), exploring surface/chemical treatments and designing new demonstrators.

[1] A. Karst, T. Parpaite, M. Bouquey, H. Pelletier, J. Soulestin, and C. Samuel, "Synthesis of PEDOT particles and manufacturing of electrically-conductive PEO / PEDOT thermoplastic composites by twin-screw extrusion," Polymer (Guildf)., vol. 290, Jan. 2024, doi: 10.1016/j.polymer.2023.126577.
[2] A. R. Jangid, E. B. Strong, J. Chuang, A. W. Martinez, and N. W. Martinez, "Evaluation of commercially-available conductive filaments for 3D printing flexible circuits on paper," PeerJ Materials Science, vol. 4, p. e21, Apr. 2022, doi: 10.7717/PEERJ-MATSCI.21.
[3] "Electrical Properties-Volume Resistivity equal 10 ohm-cm polymer product list." Accessed: Feb. 24, 2026. [Online]. Available: https://www.lookpolymers.com/findproperty.php?pid=8&sx_id=79&value=10&type=1

T. Robert : Ab initio calculated magnetic coupling between magnetic nanoparticles on graphene

Graphene (Fig.1) is a 2D material composed carbons atoms. It has exceptional electronic properties but has also few limiting properties, such has no intrinsic magnetism which can be used to encode information for example. To turn graphene in a very polyvalent and functionnalized material, one can modify its properties by proximity effect with intercalation of magnetic rare earth elements Erbium (Er) close to graphene. Such system (Fig.2) has been experimentally explored. However, this system hasn't be theoretically studied. Hence my project is on one hand to reproduce experimental results and then focus on magnetic properties and on an other hand to obtain a better understanding of the system's underlying physic. In order to reach this objective I create numerically the system and then compute interesting properties using state of the art Density Functional Theory. The latter is a method allowing to study multi-electrons systems.

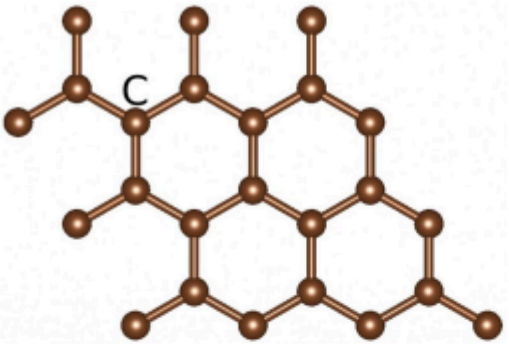


Figure 1: Graphene - top view

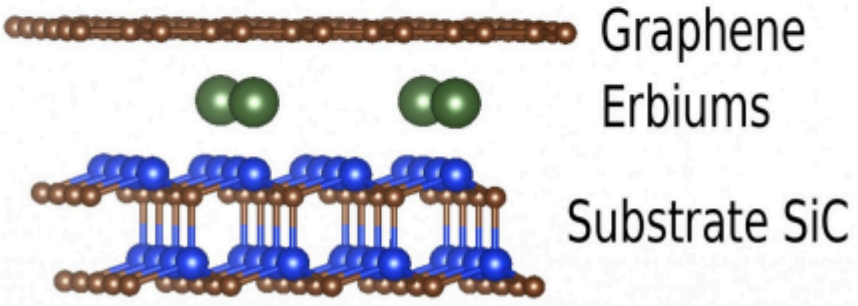


Figure 2: System - side view

S. Shetty : Electron-Hole Plasma/Liquid in suspended monolayer MoS2

Two-dimensional materials such as Transition Metal Dichalcogenides (TMDs , MoS2, WS2, etc.) exhibit strong Coulomb interactions and reduced dielectric screening, making them ideal platforms to investigate excitonic many-body physics. With sufficiently high

photoexcitation, these systems can undergo a transition from a non-interacting free exciton gas to a correlated electron-hole plasma (EHP) and eventually to a condensed electron-hole liquid (EHL). Therefore, to increase the exciton density while minimizing heat dissipation, we focus on suspended monolayers of MoS_2. We investigate the steady-state photoluminescence of suspended MoS2 as a function of the incoming laser power, using an intensity modulated beam where the exposure time (ton) and subsequent “laser off” period (toff) are tuned over a broad range spanning a few µs up to several tens of ms. Without beam modulation, we observe a large redshift of the exciton spectrum, accompanied by spectral broadening and a nonlinear increase in the integrated photoluminescence intensity. Collectively, these features indicate a phase transition from a gas of weakly interacting excitons to an EHP and ultimately EHL regime [1]. Using a modulated laser excitation, we are able to control reproducibly the onset of EHP emission. Interestingly, we observe a subtle an interplay in the spectral intensity between emission from the EHP and conventional excitonic emission. We aim to extend our studies to other TMDs and understand how the number of layers and the nature of the bandgap (direct/indirect) plays a role for the generation of EHP and EHL phases.

[1] A. W. Bataller et al., “Dense Electron − Hole Plasma Formation and Ultralong Charge Lifetime in Monolayer MoS 2 via Material Tuning,” 2019.

P. Guichard : Fast Atom Diffraction through 2D Surface

When fast atoms interact with solid surfaces, they can reveal detailed information about both the structure of the material and the interactions at play. In this project [1], we studied a new regime of fast atom diffraction in which hydrogen atoms do not reflect from a surface, but instead pass through a single layer of graphene and form a diffraction pattern. Modeling this process is particularly challenging. Hydrogen atoms are extremely light and move at very high speeds, while graphene is only one atom thick. This combination makes conventional surface-scattering models either impractical or insufficient. We developed a computational approach that makes this problem tractable while preserving the features of the atom-graphene interaction. Our results show that transmission diffraction through graphene is highly sensitive to the interaction between the hydrogen atoms and the carbon lattice. In this sense, the technique acts as an interaction spectroscopy: changes in the diffraction pattern directly reflect how the atom interacts with the material at the atomic scale. This work represents a first step toward studying fast-atom transmission diffraction in a broader range of systems. Future directions include extending the method to helium atoms and to other two-dimensional or patterned surfaces, such as hexagonal boron nitride, carbon nitride, and moiré structures, with the goal of exploring interaction phenomena in increasingly complex materials.

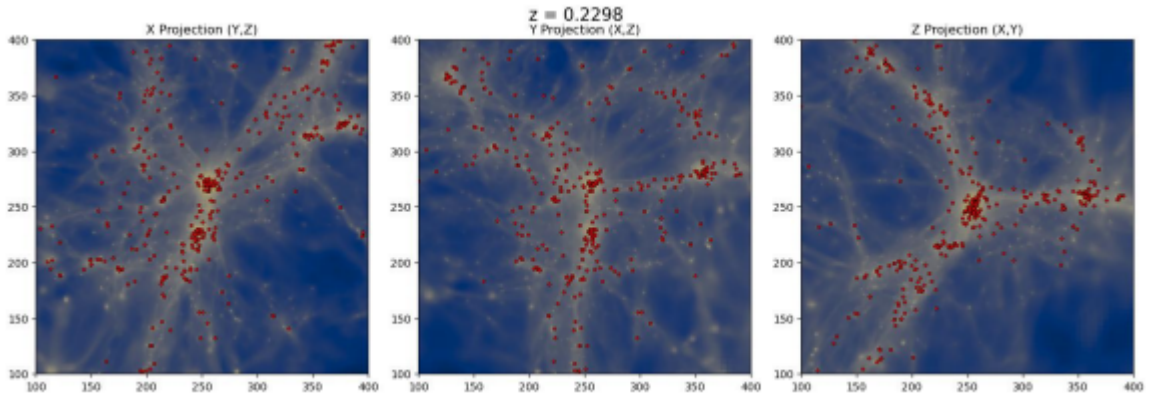
[1] P. Guichard et al, Fast Hydrogen Atom Diffraction through Monocrystalline Graphen https://journals.aps.org/prl/abstract/10.1103/wdx6-mrvm

A. Anthore : Unveiling distant galaxies with AI: Deep Learning detection of neutral hydrogen in massive radio data

The Square Kilometre Array Observatory (SKA) is the next generation of radio telescopes designed to transform our understading of the formation and evolution of galaxies. In particular, one of its key scientific goals is to trace the evolution of neutral hydrogen gas (HI) in galaxies across cosmic time. The current precursors of SKA are known to generate large, highly dimensional datasets, reaching barely the petabyte scale for most released surveys. This volume of data poses a significant challenge to classical or physics based data analysis methods. The challenge will be even greater once SKA will be operational early in the 2030s, as 700 PB of archived data per year are expected. Astronomers thus need to deelop today new scalable methods to explore such data efficiently. In this context, the objective of my PhD is to study the cosmic evolution of HI gas in and around galaxies using data from SKA precursors, in preparation of the future exploitation of SKA. This is achieved by deploying the YOLO-CIANNA method, which is a state-of-the-art deep learning method for detection and characterisation in simulated radio data, to observed radio data.

G. Aichele : To Cosmic Webs Through Neural Nets: 3D density field reconstruction from discrete tracers

During the evolution of the universe, galaxies go through multiple processes that alter their fate. It can be violent encounters with other galaxies, gravitational interactions with the surrounding gas and the internal processes of the galaxy itself. For decades, it has been interesting for astrophysicists to understand these processes, but the restriction lies in our limited ability to characterize the environments in which galaxies live. These environments are mainly identified by their density, and it is known that galaxies present in different environments have different properties such as gas distribution, temperature, rate of formation of stars and heavy element abundance (metallicity in astronomical jargon). Identifying the environments becomes hard as we look further both in distance and time, where due to the distance we miss faint objects and the environments are less defined in the earlier universe since they haven't had time to collapse gravitationally. The aim of my project is to develop a deep learning model capable of learning statistically robust representations of the universe using simulations as training data. This model should be able to build the 3D density distribution of matter using only point sources (galaxies) as the input, as can be seen on the red points displayed on top of the gas density in the figure below.



J. El Khoury : Unusual Non-linear Effects in Asymmetric Catalysis

The design of chiral catalysts presents a fundamental challenge due to the intrinsic complexity of catalytic systems. Consequently, the development of asymmetric reactions commonly begins with an empirical exploration of well-known privileged chiral structures, assuming that the active catalytic species exists as a monomer. However, since Kagan's 1986 identification of catalyst aggregation and “Non-Linear Effects” (NLEs), it has been shown that chiral structure alone is not always predictive of the system’s overall behavior, adding further intricacies to the mechanistic interpretation of asymmetric catalysis. In our study, we thoroughly examined the mechanism of the enantioselective addition of diethylzinc to benzaldehyde in the presence of the first chiral β-amino alcohol and BINOLtype ligands. The results reveal that these catalytic systems are significantly more complex than previously assumed.In the case of amino alcohols, self-induction phenomena show that the reaction can deliver higher enantiomeric excesses at lower catalyst loadings. In the systems investigated with BINOL derivatives, hyperpositive and enantiodivergent NLEs were observed, consistent with the coexistence of multiple catalytically active aggregates. Overall, these results demonstrate that these enantioselective reactions fall within the framework of Systems Chemistry

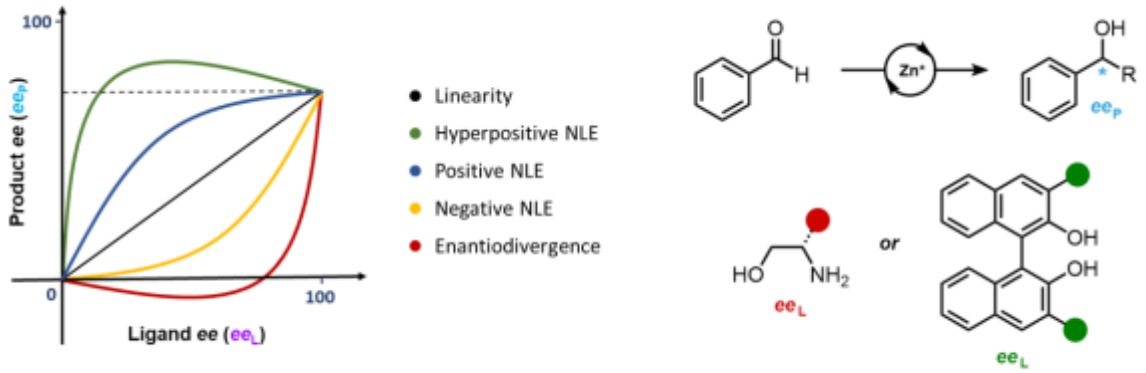


Figure 1. General scheme of non-linear effects types, the catalytic reaction and molecular structure of the chiral ligands used.

N. Zhamantay : Comprehensive TEM/STEM Analysis of High-Entropy Alloy Nanoparticles

High-entropy alloys (HEAs) are materials composed of 5 or more metals in near-equimolar proportions (5–35%). They are considered promising catalysts for the hydrogen evolution reaction (HER) and the oxygen reduction reaction (ORR). [1] In this project, we study nanoparticles composed of multiple noble and non-noble metals (such as Rh, Ru, Ir, Pt, Ni, Co and Pd) to understand how their atoms arrange and how this depends on the synthesis method. To do this, we use transmission electron microscopy (TEM), which allows us to image particles thousands of times smaller than the width of a human hair and identify their crystal structure and composition. By analyzing particle size, shape, and how the different metals are distributed, we compare well-mixed nanoparticles with others where elements separate or form different structures[2] . These observations help link the synthesis conditions with the final structure of the nanoparticles. In parallel, we are also using liquid In-situ TEM to studying the nucleation and growth of this kind of nanomaterials.

Figure 1. High Resolution TEM of Pt nanoparticle showing the crystalline planes

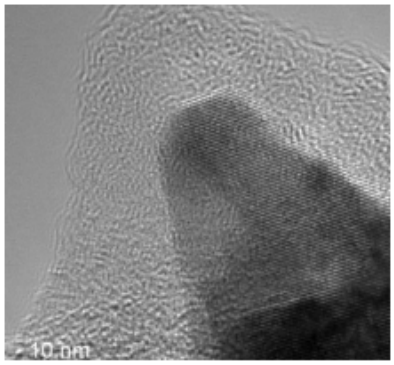
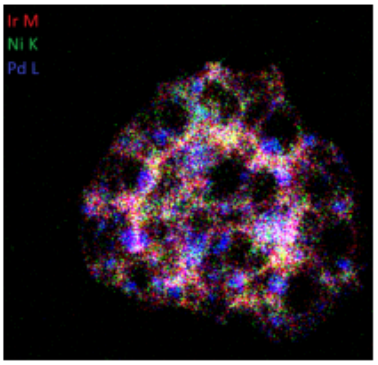


Figure 2. TEM Energy dispersive X-ray Mapping



1. George, E. P.; Raabe, D. S.; Laptev, N. J. High-Entropy Alloys. Nat. Rev. Mater. 2019, 4, 515–534.
2. De Marco, M. L.; et al. High-Entropy-Alloy Nanocrystal-Based Macro- and Mesoporous Materials for Electrocatalysis. ACS Nano 2022, 16, 15837–15849.

J. Kapp : Quinoline based luminescent imidazolium salts as vector for gene therapy

Molecular salts, particularly those based on imidazolium units, have attracted the attention of the scientific community due to their unique properties and structural versatility, especially those containing a fluorophore1,2 . Indeed, light and the phenomena associated with it, such as fluorescence, have proven to be a powerful and highly sensitive tools for exploring the nanoscale world (organization, polarity, interactions, etc.). Furthermore, cationic lipids have, for several years, emerged as the best candidates for the delivery of genetic material and thus for gene therapy3,4. In 2009, Dobbs et al 5 , had already demonstrated that the delivery of siRNA was possible using imidazolium salts. In this context, we have designed new imidazolium salts incorporating a quinoline unit in order to developed a new theragnostic agent. Thanks to the lone pair available on the nitrogen atom, quinoline is capable of interacting with protons and is therefore an ionizable unit. Our imidazolium salts are composed of three parts: a fluorophore, which is rigid and hydrophobic; the imidazolium cation, which is rigid and hydrophilic; and the alkyl chains which are flexible and hydrophobic. The combination of these three antagonist parts makes these salts a new type of highly bioavailable and luminescent molecular platform. This structural arrangement allows for fine-tuning of both the amphipathic and amphiphilic character of our salts, thereby enabling control over the emergence of their biological properties and mesomorphic properties. The quinoline ring offers seven different substitution positions, allowing the establishment of a structure–activity relationship and the supramolecular level study of the behavior of these molecules. Herein, we will present the synthesis and the study of the biological properties of these salts as a function of their substitution position on the quinoline unit.

1. Riduan, S. N.; Zhang, Y. Chem. Soc. Rev. 2013, 42, 9055–9070.
2. del Giudice, N. & al. Eur. J. Org. Chem. 2021, 2021, 2091–2098.
3. Valatabar, N. & al. J. Nanobiotechnology 2024, 22, 386.
4. Guo, X.; Huang, L. Acc. Chem. Res. 2012, 45, 971–979. 5Dobbs, W. & al. J. Am. Chem. Soc. 2009, 131, 13338–13346.